THE EFFECT OF CHANGES IN PURE COMPONENT PROPERTIES ON EQUATION OF STATE CALCULATIONS

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PREFACE

The changes in the critical temperature result in larger change in calculated results than do corresponding changes in ether critical pressure or acentric factor. The binary interaction parameter has no effect on the prediction of the pure components. However, the binary interaction parameter does have an impact on the calculated results for mixtures. The values for the physical properties originally used when the equation of state programs were written should not be changed without first recorrelating experimental data for the pure components and mixtures affected by the property changes.

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CHAPTER I

INTRODUCTION

Those interested in properties of pure components and mixtures measure and revise physical properties, such as critical temperature and pressure, of pure components. Over the years, measurement techniques, sensitivities and purification capabilities have improved. When measurements made today are compared with those made a century ago the precision and reliability of measurements made appear to have improved dramatically. For example the critical temperature of hexane is reported as 454.1 °F in 1976, 451.8 °F in 1998, the critical pressure of n-butane is reported as 550.7 psia in 1971 and 554.0 psia in 1998. The acentric factor is reported by Pitzer et al. 1955 as 0.013, Passut and Danner 1973 as 0.0072, Henry and Danner 1978 as 0.0115, and Reid et al. 1987 as 0.011.

The relationship between the pressure, volume and temperature of a gas, commonly related or expressed by what is called an equation of state, was originally formulated as the ideal gas law. The simple expression of the ideal gas law represents the behavior of actual gases as an approximation only, frequently yielding large differences between observed and calculated values for volume and/or density of real gases.

Many modifications have been suggested in order to represent more accurately the relation between the measured pressures, volumes and temperatures of a gas or liquid. Pressure and temperature are the usual properties measured and varied in experimental procedure and, from this viewpoint, are more likely to be considered the independent variables.

In recent years equations of state are increasingly being used for predicting vapor-liquid equilibrium behavior and calculating thermodynamic properties of pure components and mixtures. Desirable characteristics of an equation of state include simplicity, accuracy and applicability over a wide range of temperatures, pressures and mixture compositions. A reliable equation of state can eliminate costly and expensive laboratory investigations that might otherwise be required to obtain the data necessary for reliable design. Equations of state are widely used for natural gas and petroleum work, and increasingly are being extended to petrochemical systems.

Most equations of state require as input pure component properties such as critical temperature and pressure. There may also be need for defined parameters like the acentric factor, and even adjustable parameters like a binary interaction parameter for two components. Since the values for some of these properties change from time to time, the question comes — should the newer values replace the values originally used when the equation of state program(s) were written? That is the question this work is intended to answer.

CHAPTER II

LITERATURE REVIEW

Engineers have long utilized equations of state for calculating *PVT* relationships, vapor-liquid equilibrium and thermodynamic properties for gases and liquids. Most equations are applicable to both liquids and gases and apply to pure components and mixtures. This chapter contains a brief history and review of the development of several equations of historical significance and also of several of the many equations in use today, emphasizing those that are directly pertinent to the present study. The ideal gas, the analytical form of the van der Waals, virial expansion, Beattie and Bridgeman, Benedict-Webb-Rubin, Redlich-Kwong, Chao-Seader, Soave-Redlich-Kwong and Peng-Robinson equations are presented. Except for the virial equation, all of these equations are considered by thermodynamic purists to be empirical equations.

Ideal Gas Law

The simplest equation of state is the ideal gas, in which the molecules are assumed to be spherical, perfectly elastic and there are no intermolecular forces. The law usually appears in the form

$$PV = nRT \qquad [1]$$

Where

P = absolute pressure (atm).

V = volume (liter).

n = number of moles (gram moles).

R = universal gas constant (0.08206 liter atm/mol K).

T = absolute temperature (K).

Real gases deviate from this simple equation. However, at pressure up to a few atmospheres this equation may be considered as a good approximation for real gases.

Virial Equation

Considering the interaction of gas molecules by statistical mechanics results in an equation of state expressed as a power series expansion that is commonly referred to as the virial equation of state. The virial equation expresses the compressibility factor as a power in density (reciprocal specific volume). This power series is

$$Z = \frac{Pv}{RT} = 1 + \frac{B}{v} + \frac{C}{v^2} + \frac{D}{v^3} + \cdots \qquad [2]$$

Where

Z = compressibility factor

P = absolute pressure (atm).

v = molar volume (liter/mol).

R = universal gas constant (0.08206 liter atm/mol K).

T = absolute temperature (K).

B, C, D = virial coefficients (liter/mol)^n, n=*1, 2, 3, ...*

The parameters B, C, D, ... are called the second, third, fourth, ... etc. virial coefficients. For pure components they are functions of temperature only; for mixtures they are functions of temperature and composition; and for both must be calculated from experimental PVT measurements. In general, the virial coefficients can be correlated in terms of intermolecular forces of attraction and repulsion between molecules expressed as functions of the intermolecular distances. The virial equation forms the basis for a number of vapor-liquid equilibrium correlation and prediction methods. Often the virial equation is truncated to contain only the first and second virial coefficients. This equation is convenient to use and may be solved explicitly for volume. This equation is limited to a pressure corresponding to a density of about one-half the critical density (14). Perhaps the most important advantage of the virial equation for application to phase equilibrium problems lies in its direct extension to mixtures. The composition dependence of all virial coefficients is given by a generalization of the statistical – mechanical derivation used to derive the virial equation for pure gases. This equation of state has theoretical foundation. Perry et al 1973 stated that "The virial equation is the only equation of state based on theory" (14).

van der Wals (1873) Equation

One of the earliest equations of state was that of van der Waals (21). It is a two-constant equation that attempts to account for the influence of intermolecular forces on PVT behavior. The intermolecular attraction between the molecules as they continuously move about requires a correction to the ideal gas law calculated pressure.

The space occupied by the molecules is not all available to accommodate the motion, and the effective volume is less than the ideal gas law calculated volume. The force of attraction between molecules is called the van der Waals force. This force, by pulling the molecules together, reduces the pressure below the value calculated from ideal-gas principles. Kinetic theory shows this pressure to be inversely proportional to the square of the molar volume. Using these observations the van der Waals equation has been derived as

$$P = \frac{RT}{v-b} - \frac{a}{v^2} \qquad [3]$$

Where

a , b = correlation constants.

P = absolute pressure (atm).

v = molar volume (liter/mol).

R = universal gas constant (0.08206 liter atm/mol K).

T = absolute temperature (K).

a and b are characteristics of each gas and are called the van der Waals constants. These constants have been determined to be dependent on temperature and the density of the fluid. They can be calculated from critical properties by applying the van der Waals equation to the critical point. Usually values for the van der Waals constants are calculated from critical pressure and temperature. The van der Waals equation provides a logical starting point for many modifications. The van der Waals type equations of state currently in use resemble their common predecessor in that all of them contain a repulsive term and an attractive term. In equation [3] the repulsive part is represented by $RT/(v-b)$ and the attractive part by a/v^2.

Beattie-Bridgeman (1928) Equation

Beattie and Bridgeman (2) gave a theoretical basis for their equation and a detailed method for obtaining the constants from *PVT* data. Assuming that the measured pressure of a gas can be written as the difference of two terms, one of which arises from the kinetic energy of the gas the other from its potential energy, the proposed equation is

$$p = \frac{RT(1 - c/VT^3)}{V^2}[V + B_0(1 - b/V)] - \frac{A_0}{V^2}(1 - \frac{a}{V}) \qquad [4]$$

Where

P = pressure (atm).

T = temperature (K).

V = molar volume (liter/mol).

R = gas constant (0.8206 liter atm/mol K)

A_0, B_0, a, b, and c are constants whose values depend upon the kind of gas under consideration. Beattie and Bridgeman evaluated the constants and tested their equation against experimental *PVT* measurements for ten gases (helium, neon, argon, hydrogen, nitrogen, oxygen, air, carbon dioxide, methane and ether). The average deviation was 0.18 % between the calculated and observed pressures (2). With the exception of c, each of the constants appears as the slope or intercept of a straight line plot of the data. The constant c was determined from the mean curvature between two sets of isometric data. Beattie and Bridgeman indicated in their paper that the region immediately around the critical point is not considered and the position of the ice point is taken as 273.13° K.

Benedict-Webb-Rubin (1940) Equation

The Benedict-Webb-Rubin (3) equation was derived as an improvement on the Beattie-Bridgeman equation. This empirical equation defines the pressure as a polynomial equation in density with coefficients that are temperature dependent. Experimental *PVT* data along with critical properties, and vapor pressures were used to determine the eight parameters (4). This equation is

$$P = TRd + (B_0RT - A_0 - C_0/T^2)d^2 + (bRT - a)d^3 + a\alpha d^6 + \frac{cd^3(1+\gamma d^2)\exp(1-\gamma d^2)}{T^2} \quad [5]$$

Where

P = pressure (atm).

T = temperature (taken as 273.13 K).

d = molar density (mol/liter).

R = universal gas constant (taken as 0.08207 liter atm/mol K).

A procedure is suggested for determining numerical values of the parameters by expressing the dependence of, A_0, B_0, C_0 on density by linear equations and adjusting the values of a, b, c, γ, and α to give the best representation of observed vapor pressure

Redlich-Kwong (1949) Equation

Redlich and Kwong (17) proposed the first cubic equation of state that was widely accepted and used as a tool for routine engineering calculations. It has only two parameters. The term "cubic equation of state" describes an equation which, if expanded, would contain volume terms raised to the third power. The RK equation has retained its popularity of use over the years, and there have been a number of modifications.

The equation is

$$P = \frac{RT}{(V-b)} - \frac{a}{T^{1/2}V(V+b)} \qquad [6]$$

Where

$$a = 0.4278\, R^2\, T_c^{2.5}/P_c \qquad [7]$$

$$b = 0.0867\, R\, T_c/P_c \qquad [8]$$

P = pressure (atm).

V = molar volume (liter/mol).

R = universal gas constant (0.08206 liter atm /mol K).

T = absolute temperature (K)

The equation has been constructed to satisfy the condition $b = 0.26\, V_c$ in order to get good approximation of experimental data at high pressure (17). The criteria that the first and the second partial derivatives of pressure with respect to the volume are zero at the critical point is used to evaluate the parameters a and b as a functions of the critical temperature and critical pressure of the component. The constants a and b can be most accurately determined by fitting the constants using experimental PVT data. The success and wide use of the Redlich-Kwong equation of state stimulated numerous investigators to propose various methods for improving it.

Chao-Seader (1961) Equation

The Chao-Seader equation has the distinction of being the first equation of state developed using a computer, and intended for solution using a computer. In the Chao-Seader (5) equation the vapor-liquid equilibrium ratio (K-value) of any component, i, in a mixture is computed from a combination of three factors: the activity coefficient of component i in the liquid mixture, the fugacity coefficient of component i in the vapor mixture and the fugacity coefficient of pure liquid i at system conditions.

$$K_i \equiv \frac{y_i}{x_i} \equiv v_i^0 \frac{\gamma_i}{\phi_i} \qquad [9]$$

Where

K_i = vapor-liquid equilibrium constant of component *i*.

y_i = mole fraction of component *i* in vapor mixture.

x_i = mole fraction of component *i* in liquid solution.

γ_i = activity coefficient of component *i* in liquid solution.

ϕ_i = fugacity coefficient of component *i* in vapor mixture.

v_i^0 = fugacity coefficient of pure liquid of component *i* at system conditions.

The fugacity coefficient v^o of a pure liquid component at system conditions is correlated within the framework of Pitzer's modified form of the principle of corresponding states which states that substances at equal reduced pressures and temperatures are assumed to have equal reduced volumes. The activity coefficient of component *i* in liquid solution γ_i is calculated from Hildebrand's equation in which the solubility parameter is defined as the square root of an energy density with regular liquid solution assumed. A solution that has an excess entropy of zero is called a regular solution. The fugacity coefficient of component *i* in vapor mixture ϕ_i is calculated from the Redlich-Kwong equation of state. The correlation applies to hydrocarbons of various types, including paraffins, olefins, aromatics and naphthenes. Gaseous hydrogen dissolved in hydrocarbon mixtures is likewise correlated. The correlation has been tested with literature data on mixtures of these compounds with an overall average deviation of 8.7% (5).

The Soave-Redlich-Kwong (1972) Equation

Soave (19) proposed a modification to the Redlich-Kwong equation by assuming the parameter a in the original equation to be temperature-dependent, and introducing the acentric factor as a third parameter. The term $a/T^{0.5}$ in equation [6] was replaced with a more temperature dependent term $a\ (T, \omega)$. This equation is

$$p = \frac{RT}{v-b} - \frac{a(T)}{v(v+b)} \qquad [10]$$

Where

$$a_{ci} = 0.42747\, R^2\, T_{ci}^{\,2}/P_{ci} \qquad [11]$$

$$b_i = 0.08664\, R\, T_{ci}/P_{ci} \qquad [12]$$

$$a_i\,(T) = a_{ci}\ \alpha_i\,(T) \qquad [13]$$

$$\alpha_i^{0.5} = 1 + m_i\,(1 - T_{ri}^{\,0.5}) \qquad [14]$$

$$m_i = 0.480 + 1.57\ \omega_i - 0.176\ \omega_i^2 \qquad [15]$$

p = absolute pressure (psia)

T = absolute temperature (°R).

R = universal gas constant (10.73 ft^3 psia/lb-mole °R).

v = molar volume (ft^3/lb-mole).

a, b = equation parameters.

ω = acentric factor

T_c = critical temperature (°R).

P_c = critical pressure (psia).

T_R = reduced temperature (T/T_c)

P_R = reduced pressure (P/P_c)

a_c = value of $a(T)$ at $T=T_c$

m = slope of $\alpha^{0.5}$ against $T_R^{0.5}$

Expressing the temperature dependence as in equations [11] through [15], where m is expressed as a quadratic function of the acentric factor, has gained widespread popularity due to its simplicity. Soave obtained his relation by forcing the equation to reproduce vapor pressure for nonpolar substances at $Tr = 0.7$.

Peng-Robinson (1976) Equation

The Peng-Robinson (13) equation of state was developed by using the same bases as the Soave equation. Recognizing that the critical compressibility factor of the SRK equation of state (Z_c=0.333) is overestimated, thus impairing the liquid volume calculations, they postulated an equation reducing Z_c to 0.307. This improved the representation of liquid density in relation to the SRK.

$$P = \frac{RT}{v-b} - \frac{a(T)}{v(v+b)+b(v-b)} \qquad [16]$$

Where

$$a(T_c) = 0.45724\, R^2 T_c^2 / P_c \qquad [17]$$

$$b(T_c) = 0.07780\, RT_c / P_c \qquad [18]$$

$$a(T) = a(T_c)\, \alpha\,(T_r, \omega) \qquad [20]$$

$$b(T) = b(T_c) \qquad [21]$$

$$\alpha^{1/2} = 1 + \kappa(1 - T_r^{1/2}) \qquad [22]$$

$$\kappa = 0.37464 + 1.54226\, \omega - 0.26992\, \omega^2 \qquad [23]$$

p = absolute pressure (psia)

T = absolute temperature (°R).

R = universal gas constant (10.73 ft^3 psia/lb-mole °R).

v = molar volume (ft^3/lb-mole).

a, b = equation parameters.

ω = acentric factor

T_c = critical temperature (°R).

P_c = ctitical pressure (psia).

T_R = reduced temperature (T/T_c)

P_R = reduced pressure (P/P_c)

a_c = value of $a(T)$ at $T=T_c$

m = slope of $\alpha^{0.5}$ against $T_R^{0.5}$

The Soave-Redlich-Kwong (SRK) and Peng-Robinson (PR) equations of state are the most widely used and have enjoyed considerable success in their application because of their simplicity and reasonable accuracy when dealing with hydrocarbon mixtures. Many attempts have been made to increase the reliability of the SRK and the PR. These can be broadly classified as attempts to improve the estimation of pure fluid properties, modify the mixing rules, and generalize the binary interaction parameters.

Mixing Rules

The most widely used method for extending equations of state to mixtures is to use the classical one-fluid approach. In this approach, the properties of a fluid mixture are assumed to be the same as those of a hypothetical pure fluid at the same temperature and pressure but having the characteristic constants appropriately averaged over the composition. The averaging functions (mixing rules) are quadratic in mole fraction.

$$a_m = \Sigma\Sigma x_i x_j a_{ij} \quad [24]$$

$$b_m = \Sigma x_i b_i \quad [25]$$

$$a_{ij} = (1-k_{ij}) a_i^{1/2} a_j \, ½ \quad [26]$$

Where

a_m = the a parameter for the mixture.

b_m = the b parameter for the mixture.

a_i, a_j, b_i = a and b parameters for any components in the mixture.

x_i, x_j = composition (mole fraction) for any two components in the mixture.

k_{ij} = binary interaction parameter.

Even though the mixing rules stated in equations [24] though [26] are most commonly used, other mixing rules have been proposed over the years (5), (11). However, the simplicity of the classical mixing rules with one or two binary interaction parameters make them attractive to equation of state developers. The performance of the classical mixing rules was thoroughly tested for several equations of state by Tsonopoulos and Heidman 1986. The pure component parameters are generalized in terms of the critical temperature, critical pressure and acentric factor.

Pitzer's Acentric Factor (1955)

Pitzer (15) postulated that the slope of the reduced vapor pressure curve is the most sensitive property for a third parameter base. Since vapor pressure can be measured with better accuracy than critical properties, this approach should be superior to using the critical compressibility factor (16). Pitzer defined the acentric factor ω as

$$\omega = -\log P_r - 1.000 \qquad [29]$$

where P_r is the reduced vapor pressure at $T_r = 0.70$. This particular form was chosen to ensure that $\omega = 0.0$ for spherical noble gases, while other fluids will have some other value of ω. Pitzer (16) reported that the reduced vapor pressure for the "simple fluids" Argon, Krypton Zenon and Methane is almost 0.1 at a reduced temperature of 0.7. This value of reduced temperature was taken to be the standard point for determining the acentric factor which is defined in equation [29].

From the definition of the acentric factor, the accuracy of its value clearly depends upon the accuracy of available values for the vapor pressure, critical temperature and critical pressure.

The value of the acentric factor from this procedure certainly depends on the type of vapor pressure equation employed and the source of vapor pressure data used. For example, for the simple gas methane the value of the acentric factor has been reported by Pitzer et al. 1955 as 0.013, Passut and Danner 1973 as 0.0072, Henry and Danner 1978 as 0.0115, and Reid et al. 1987 as 0.011.

CHAPTER III

METHODOLOGY

Equation of state models require the use of pure component properties like critical temperature and pressure and acentric factor. Such properties must be available if most equations of state are to be used for prediction of physical and thermodynamic properties for pure components and mixtures. Over the years, measurement techniques, sensitivities and capabilities have improved incrementally. When measurements made today are compared with those made a century ago the reported properties in many cases have changed significantly with the passage of time. This raises the question, "Should the newer values replace the values originally used when the equation of state program was written?" To answer this question, one needs to know how changes in these properties change the values calculated by the equation of state. The work reported here answers this question.

The equations of state studied were the Soave-Redlich-Kwong (SRK) (19) and the Peng-Robinson (PR) (13). They were selected because each is widely used in industrial work, and versions of them are available in most commercial process simulators, making them available to most practicing engineers.

The specific program used (EZ-THERMO) is based on the SRK equation of state and was developed by Moshfeghian and Maddox (9). The original version of this package called "Microsim" was developed by Erbar and Maddox (8) with additions and adjustments for new operating systems and computers by Maddox and Shariat (7). The program has been in continuous use for more than 25 years. When first written it was tested against all available experimental data for the 61 components on its data base. There is a continuous program of evaluation as new experimental data are published. Conservative estimates are that 100+ man years have been devoted to evaluation and testing of the program. The computer programs as written were modified to allow the user to make changes in the pure component properties including critical temperature, critical pressure and acentric factor. A separate modification to the SRK program allowed changes in the binary interaction parameter for the mixture studies.

Changes in critical temperature, critical pressure and the acentric factor were made for a variety of light hydrocarbons ranging from methane to heptane. Pure components were studied at the bubble point and dew point, binary mixtures were studied at the bubble point, dew point and 50% liquid flash, and multicomponent mixtures were flashed at 100 psia and 100 °F to produce 50% liquid and also to determine the effects of the binary interaction parameter. The first systems studied were pure components at the bubble point and dew point. This was followed by studies of several binary mixtures and finally by multicomponent mixtures.

For a single component at saturation conditions the vapor-liquid equilibrium constant is always exactly 1.0. For many cases an equation of state like the SRK will reach an apparently satisfactory solution. Close inspection will show that equilibrium

constants for all components are 1.0 within a very small error limit. Something is needed to detect this kind of "solution". Introducing a second component, even at zero concentration solves this problem. As can be seen in Tables IA, IIA in Appendix A, the second component K-value is clearly different from 1.0 when a valid solution is reached.

Changes made in critical temperature, critical pressure and acentric factor are in small, uniform increments. Percentage change does not make sense in this work because of the range of critical temperature, critical pressure and acentric factor encountered. Consider a change in critical temperatue of 5 K. This is about 2.5% of the critical temperature for methane. For heptane the 5 K increment is only about 0.5% and for heavier hydrocarbons it will be even less.

CHAPTER IV

RESULTS

a) Pure Component

Bubble point temperature and dew point temperature calculations at 100 psia (698.48 kPa) for methane, ethane, propane and n-butane were performed using the SRK and the PR equations of state. Arbitrary changes in critical temperature, critical pressure and acentric factor were made for each of the pure hydrocarbons. Calculations were carried out to see how the changes in pure component properties influenced the calculation results. Property changes were made in both the liquid (bubble point calculations) and vapor (dew point) phases. In all tables the bolded numbers indicate values currently used in the equation of state.

Methane Bubble Point Calculations

The effect of changing the critical temperature on the calculated bubble point for methane is shown in Table I (a). Increasing the critical temperature by 1 °F, increases the calculated bubble point for methane by 0.74°F for the SRK and by 0.75 for the PR. Increasing the critical temperature by 5°F, increases the bubble point temperature by 3.7 °F for the SRK and by 3.71 °F for the PR. Lowering the critical temperature lowers the calculated bubble point by almost the same amount.

Worth mention at this point is that rounding and truncating numbers is necessary to provide fixed decimal output in the equation of state results. In the case above 0.74 and 0.75 as well as 3.70 and 3.71 are considered to be the same number for purposes of comparing results.

Table II (a) shows the result of changing methane critical pressure on the calculated bubble point. Results for both equations are again similar, but the change is much smaller. An increase in critical pressure of 5 psia, decreases the calculated bubble point temperature by only 0.26 °F for both the SRK and the PR. Lowering the critical pressure increases the calculated bubble point temperature by almost the amount (3.7 °F).

Table I (a). Effect of Change in Critical Temperature on Calculated Bubble Point of Methane.

Critical Temperature T (°F)	Bubble Point Temperature (°F)		Enthalpy (kBTU)*	
	SRK	PR	SRK	PR
-111.63	-202.13	-201.47	-130.32	-128.58
-112.63	-202.87	-202.21	-129.95	-128.22
-113.63	-203.61	-202.95	-129.59	-127.86
-114.63	-204.35	-203.69	-129.23	-127.51
-115.63	-205.09	-204.43	-128.87	-127.15
-116.63	**-205.83**	**-205.18**	**-128.50**	**-126.79**
-117.63	-206.57	-205.92	-128.14	-126.43
-118.63	-207.31	-206.66	-127.78	-126.07
-119.63	-208.05	-207.40	-127.41	-125.72
-120.63	-208.79	-208.14	-127.05	-125.36
-121.63	-209.53	-208.89	-126.69	-125.00

* kBTU means thousands of BTU

Table II (a). Effect of Change in Critical Pressure on Calculated Bubble Point of Methane.

Critical Pressure P (psia)	Bubble Point Temperature (°F)		Enthalpy (kBTU)	
	SRK	PR	SRK	PR
672.75	-206.09	-205.44	-128.92	-127.19
671.75	-206.04	-205.39	-128.84	-127.11
670.75	-205.99	-205.33	-128.75	-127.03
669.75	-205.93	-205.28	-128.67	-126.95
668.75	-205.88	-205.23	-128.59	-126.87
667.75	**-205.83**	**-205.18**	**-128.50**	**-126.79**
666.75	-205.78	-205.12	-128.42	-126.71
665.75	-205.72	-205.07	-128.33	-126.63
664.75	-205.67	-205.02	-128.25	-126.55
663.75	-205.62	-204.96	-128.17	-126.46
662.75	-205.56	-204.91	-128.08	-126.38

Increasing the acentric factor from (**0.0039** to 0.0049) increases the bubble point temperature by 0.07 °F for the SRK. Increasing the acentric factor for the PR from (**0.014** to 0.024) increases the bubble point temperature by 0.67 °F. The results are shown in Table III (a).

Table III (a). Effect of Changes in Acentric Factor on Calculated Bubble Point of Methane.

Acentric Factor ω	Bubble Point Temperature T (°F)	Enthalpy (kBTU)	Acentric Factor ω	Bubble Point Temperature T (°F)	Enthalpy (kBTU)
SRK	SRK	SRK	PR	PR	PR
0.00890	-205.51	-130.03	0.0640	-201.98	-142.45
0.00790	-205.57	-129.72	0.0540	-202.60	-139.32
0.00690	-205.63	-129.42	0.0440	-203.23	-136.19
0.00590	-205.70	-129.11	0.0340	-203.86	-133.06
0.00490	-205.76	-128.81	0.0240	-204.51	-129.93
0.00390	**-205.83**	**-128.50**	**0.0140**	**-205.18**	**-126.79**
0.00290	-205.89	-128.20	0.0040	-205.85	-123.65
0.00190	-205.96	-127.89	0.0030	-205.92	-123.34
0.00090	-206.02	-127.59	0.0020	-205.99	-123.02
0.00001	-206.08	-127.35	0.0010	-206.06	-122.71

Methane Dew Point Calculations

The effect of changing the critical temperature on the calculated dew point for methane is shown in Table IV (a). Increasing the critical temperature by 1 °F, increases the calculated dew point for methane by 0.74 °F for the SRK and by 0.75 °F for the PR. Increasing the critical temperature by 5 °F, increases the dew point temperature by 3.7 °F for the SRK and by 3.72 °F for PR. Lowering the critical temperature by 5 °F lowers the calculated dew point by almost the same amount.

Table IV (a). Effect of Change in Critical Temperature on Calculated Dew Point of Methane.

Critical Temperature T (°F)	Dew Point Temperature (°F)		Enthalpy (kBTU)	
	SRK	PR	SRK	PR
-111.63	-202.13	-201.46	182.08	182.35
-112.63	-202.87	-202.21	181.54	181.81
-113.63	-203.61	-202.95	181.00	181.28
-114.63	-204.35	-203.69	180.47	180.74
-115.63	-205.09	-204.43	179.94	180.21
-116.63	**-205.83**	**-205.18**	**179.40**	**179.67**
-117.63	-206.57	-205.92	178.87	179.14
-118.63	-207.31	-206.66	178.33	178.60
-119.63	-208.05	-207.40	177.80	178.07
-120.63	-208.79	-208.14	177.26	177.53
-121.63	-209.53	-208.88	176.73	176.99

Table V (a) shows the results of changing methane critical pressure on the calculated dew point. Results for both equations are again similar, but the changes are much smaller. An increase in critical pressure of 5 psia, decreases the calculated dew point of only 0.26 °F for both the SRK and the PR. Lowering the critical pressure by 5 psia, increases the calculated dew point by almost the same amount.

Changing the critical pressure by one psia, (from **667.75** to 668.75 psia), decreases the dew point calculation by 0.05 °F for both the SRK and the PR. These results are show in Table V (a).

Changing the acentric factor from (**0.0039** to 0.0049) increases the dew point temperature by 0.07 °F for the SRK. Changing the acentric factor for the PR from (**0.014** to 0.024) increases the dew point temperature by 0.67 °F. The results are shown in Table VI (a).

Table V (a). Effect of Change in Critical Pressure on Calculated Dew Point of Methane.

Critical Pressure P (psia)	Dew Point Temperature (°F)		Enthalpy (kBTU)	
	SRK	PR	SRK	PR
672.75	-206.09	-205.44	179.31	179.58
671.75	-206.04	-205.38	179.33	179.60
670.75	-205.98	-205.33	179.35	179.62
669.75	-205.93	-205.28	179.36	179.63
668.75	-205.88	-205.23	179.38	179.65
667.75	**-205.83**	**-205.18**	**179.40**	**179.67**
666.75	-205.77	-205.12	179.42	179.69
665.75	-205.72	-205.07	179.44	179.71
664.75	-205.67	-205.01	179.46	179.73
663.75	-205.61	-204.96	179.47	179.74
662.75	-205.56	-204.91	179.49	179.76

Table VI (a). Effect of Changes in Acentric Factor on Calculated Dew Point of Methane.

Acentric Factor ω	Dew Point Temperature T (°F)	Enthalpy (kBTU)	Acentric Factor ω	Dew Point Temperature T (°F)	Enthalpy (kBTU)
SRK	SRK	SRK	PR	PR	PR
0.00890	-205.50	179.60	0.0640	-201.98	181.68
0.00790	-205.57	179.56	0.0540	-202.60	181.29
0.00690	-205.63	179.52	0.0440	-203.22	180.90
0.00590	-205.70	179.48	0.0340	-203.86	180.50
0.00490	-205.76	179.44	0.0240	-204.51	180.09
0.00390	**-205.83**	**179.40**	**0.0140**	**-205.18**	**179.67**
0.00290	-205.89	179.36	0.0040	-205.85	179.24
0.00190	-205.96	179.32	0.0030	-205.92	179.20
0.00090	-206.02	179.28	0.0020	-205.98	179.16
0.00001	-206.08	179.24	0.0010	-206.05	179.11

Ethane Bubble Point Calculations

The effect of changing the critical temperature on the calculated bubble point for ethane is shown in Table VII (a). Increasing the critical temperature by 1 °F, increases the calculated bubble point for ethane by 0.75°F for the SRK and by 0.76°F for the PR. Increasing the critical temperature by 5 °F, increases the bubble point temperature by 3.75 °F for the SRK and by 3.76 for the PR. Lowering the critical temperature lowers the calculated bubble point by almost the same amount.

Table VII (a). Effect of Change in Critical Temperature on Calculated Bubble Point of Ethane.

Critical Temperature T (°F)	Bubble Point Temperature (°F)		Enthalpy (kBTU)	
	SRK	PR	SRK	PR
95.09	-43.48	-42.70	-210.25	-205.63
94.09	-44.23	-43.45	-210.03	-205.42
93.09	-44.98	-44.20	-209.81	-205.21
92.09	-45.73	-44.95	-209.59	-205.00
91.09	-46.48	-45.70	-209.37	-204.78
90.09	**-47.23**	**-46.46**	**-209.15**	**-204.57**
89.09	-47.98	-47.21	-208.92	-204.35
88.09	-48.73	-47.96	-208.70	-204.14
87.09	-49.48	-48.71	-208.48	-203.92
86.09	-50.23	-49.46	-208.25	-203.71
85.09	-50.98	-50.21	-208.02	-203.49

Table VIII (a) shows the result of changing ethane critical pressure on the calculated bubble point. Results for both equations are again similar, but the change is much smaller than for changing critical temperature. An increase in critical pressure of 5 psia, decreases the calculated bubble point temperature of only 0.37 °F for both the SRK and the PR. Lowering the critical pressure increases the calculated bubble point by almost the same amount. Increasing the critical pressure by one psi, decreases the calculated bubble point calculation by 0.07 °F for both the SRK and PR. These results are shown in Table VIII (a).

Table VIII (a). Effect of Change in Critical Pressure on Calculated Bubble Point of Ethane.

Critical Pressure P (psia)	Bubble Point Temperature (°F)		Enthalpy (kBTU)	
	SRK	PR	SRK	PR
712.78	-47.60	-46.83	-209.92	-205.32
711.78	-47.53	-46.75	-209.77	-205.17
710.78	-47.45	-46.68	-209.61	-205.02
709.78	-47.38	-46.61	-209.46	-204.87
708.78	-47.31	-46.53	-209.30	-204.72
707.78	**-47.23**	**-46.46**	**-209.15**	**-204.57**
706.78	-47.16	-46.38	-208.99	-204.42
705.78	-47.08	-46.30	-208.83	-204.27
704.78	-47.01	-46.23	-208.68	-204.11
703.78	-46.93	-46.15	-208.52	-203.96
702.78	-46.86	-46.08	-208.36	-203.81

Changing the acentric factor from (**0.0944** to 0.1044) increases the bubble point temperature of ethane by 0.9 °F for the SRK. Changing the acentric factor for the PR from (**0.09947** to 0.10947) increases the bubble point temperature by 0.93 °F. The results are shown in Table IX (a).

Table IX (a). Effect of Changes in Acentric Factor on Calculated Bubble Point of Ethane.

Acentric Factor ω	Bubble Point Temperature T (°F)	Enthalpy (kBTU)	Acentric Factor ω	Bubble Point Temperature T (°F)	Enthalpy (kBTU)
SRK	SRK	SRK	PR	PR	PR
0.14440	-42.84	-232.44	0.14947	-41.97	-228.22
0.13440	-43.69	-227.77	0.13947	-42.84	-223.50
0.12440	-44.56	-223.11	0.12947	-43.72	-218.77
0.11440	-45.44	-218.46	0.11947	-44.62	-214.04
0.10440	-46.33	-213.80	0.10947	-45.53	-209.31
0.09440	**-47.23**	**-209.15**	**0.09947**	**-46.46**	**-204.57**
0.08440	-48.15	-204.50	0.08947	-47.40	-199.83
0.07440	-49.08	-199.85	0.07947	-48.36	-195.09
0.06440	-50.03	-195.21	0.06947	-49.34	-190.34
0.05440	-50.00	-190.56	0.05947	-50.33	-185.59
0.04440	-51.98	-185.93	0.04947	-51.34	-180.85

Ethane Dew Point Calculations

The effect of changing the critical temperature on the calculated dew point for ethane is shown in Table X (a). Increasing the critical temperature by 1 °F, increases the calculated dew point for ethane by 0.75 °F for the SRK and by 0.76 °F for the PR. Increasing the critical temperature by 5 °F, increases the dew point temperature by 3.75 °F for the SRK and by 3.76 for the PR. Lowering the critical temperature lowers the calculated dew point by almost the same amount.

Table X (a). Effect of Change in Critical Temperature on Calculated Dew Point of Ethane.

Critical Temperature T (°F)	Dew Point Temperature (°F)		Enthalpy (kBTU)	
	SRK	PR	SRK	PR
95.09	-43.48	-42.70	342.43	342.97
94.09	-44.23	-43.45	341.65	342.19
93.09	-44.98	-44.20	340.87	341.41
92.09	-45.73	-44.95	340.10	340.63
91.09	-46.48	-45.70	339.32	339.86
90.09	**-47.23**	**-46.46**	**338.55**	**339.08**
89.09	-47.98	-47.21	337.78	338.31
88.09	-48.73	-47.96	337.00	337.53
87.09	-49.48	-48.71	336.23	336.76
86.09	-50.23	-49.46	335.46	335.99
85.09	-50.98	-50.21	334.69	335.22

Table XI (a) shows the result of changing ethane critical pressure on the calculated dew point. Results for both equations are again similar, but the changes are much smaller. An increase in critical pressure of 5 psia, decreases the calculated dew point by only 0.37 °F for both the SRK and the PR.

Lowering the critical pressure increases the calculated dew point by almost the same amount. Changing the critical pressure by one psi, decreases the dew point calculation by 0.07 °F for both the SRK and the PR. These results are shown in Table XI (a).

Table XI (a). Effect of Change in Critical Pressure on Calculated Dew Point of Ethane.

Critical Pressure P (psia)	Dew Point Temperature (°F)		Enthalpy (kBTU)	
	SRK	PR	SRK	PR
712.78	-47.60	-46.83	338.32	338.85
711.78	-47.53	-46.75	338.36	338.90
710.78	-47.45	-46.68	338.41	338.94
709.78	-47.38	-46.60	338.46	338.99
708.78	-47.31	-46.53	338.50	339.04
707.78	**-47.23**	**-46.46**	**338.55**	**339.08**
706.78	-47.16	-46.38	338.60	339.13
705.78	-47.08	-46.30	338.64	339.18
704.78	-47.01	-46.23	338.69	339.22
703.78	-46.93	-46.15	338.74	339.27
702.78	-46.86	-46.08	338.78	339.32

Changing the acentric factor from (**0.0944** to 0.1044) increases the dew point temperature by 0.9 °F for the SRK. Changing the acentric factor for the PR from (**0.09947** to 0.10947) increases the dew point temperature by 0.93 °F. The results are shown in Table XII (a).

Table XII (a). Effect of Changes in Acentric Factor on Calculated Dew Point of Ethane.

Acentric Factor ω	Dew Point Temperature T (°F)	Enthalpy (kBTU)	Acentric Factor ω	Dew Point Temperature T (°F)	Enthalpy (kBTU)
SRK	SRK	SRK	PR	PR	PR
0.14440	-42.84	342.63	0.14947	-41.97	343.26
0.13440	-43.69	341.84	0.13947	-42.84	342.46
0.12440	-44.56	341.04	0.12947	-43.72	341.63
0.11440	-45.44	340.22	0.11947	-44.62	340.80
0.10440	-46.33	339.39	0.10947	-45.53	339.95
0.09440	**-47.23**	**338.55**	**0.09947**	**-46.46**	**339.08**
0.08440	-48.15	337.69	0.08947	-47.40	338.20
0.07440	-49.08	336.82	0.07947	-48.36	337.30
0.06440	-50.03	335.93	0.06947	-49.33	336.39
0.05440	-51.00	335.03	0.05947	-50.33	335.45
0.04440	-51.98	334.11	0.04947	-51.34	334.50

Propane Bubble Point Calculations

The effect of changing the critical temperature on the calculated bubble point for propane is shown in Table XIII (a). Increasing the critical temperature by 1 °F, increases the calculated bubble point for propane by 0.77°F for both the SRK and the PR. Increasing the critical temperature by 5°F, increases the bubble point temperature by 3.86 °F for both the SRK and the PR. Lowering the critical temperature lowers the calculated bubble point by almost the same amount.

Table XIII (a). Effect of Change in Critical Temperature on Calculated Bubble Point of Propane.

Critical Temperature T (°F)	Bubble Point Temperature (°F)		Enthalpy (kBTU)	
	SRK	PR	SRK	PR
211.01	58.18	59.18	-131.26	-125.23
210.01	57.41	58.41	-131.54	-125.53
209.01	56.64	57.64	-131.82	-125.82
208.01	55.87	56.86	-132.10	-126.11
207.01	55.09	56.09	-132.37	-126.39
206.01	**54.32**	**55.32**	**-132.65**	**-126.68**
205.01	53.55	54.54	-132.92	-126.97
204.01	52.78	53.77	-133.19	-127.25
203.01	52.00	52.99	-133.47	-127.53
202.01	51.23	52.22	-133.74	-127.81
201.01	50.46	51.45	-134.00	-128.09

Table XIV (a) shows the results of changing propane critical pressure on the calculated propane bubble point. Results for both equations are again similar, but the change is much smaller. An increase in critical pressure of 5 psia, decreases the calculated bubble point temperature by only 0.52 °F for the SRK and by 0.53 °F for the PR. Lowering the critical pressure increases the calculated bubble point by almost the same amount. Increasing the critical pressure by one psi, decreases the calculated bubble point by 0.10 °F for both the SRK and the PR. These results are shown in Table XIV (a).

Table XIV (a). Effect of Change in Critical Pressure on Calculated Bubble Point of Propane.

Critical Pressure P (psia)	Bubble Point Temperature (°F)		Enthalpy (kBTU)	
	SRK	PR	SRK	PR
621.35	53.80	54.79	-134.17	-128.17
620.35	53.91	54.90	-133.86	-127.88
619.35	54.01	55.00	-133.56	-127.58
618.35	54.11	55.11	-133.26	-127.28
617.35	54.22	55.21	-132.95	-126.98
616.35	**54.32**	**55.32**	**-132.65**	**-126.68**
615.35	54.43	55.42	-132.34	-126.38
614.35	54.53	55.53	-132.04	-126.08
613.35	54.63	55.63	-131.73	-125.78
612.35	54.74	55.74	-131.42	-125.48
611.35	54.85	55.84	-131.11	-125.17

Changing the acentric factor from (**0.1497** to 0.1597) increases the calculated propane bubble point temperature by 0.96 °F for the SRK. Increasing the acentric factor for the PR from (**0.15355** to 0.16355) increases the bubble point temperature by 0.97 °F. The results are shown in Table XV (a).

Table XV (a). Effect of Changes in Acentric Factor on Calculated Bubble Point of Propane.

Acentric Factor ω	Bubble Point Temperature T (°F)	Enthalpy (kBTU)	Acentric Factor ω	Bubble Point Temperature T (°F)	Enthalpy (kBTU)
SRK	SRK	SRK	PR	PR	PR
0.19970	58.99	-157.21	0.20355	60.05	-151.44
0.18970	58.09	-152.28	0.19355	59.13	-146.49
0.17970	57.17	-147.36	0.18355	58.20	-141.53
0.16970	56.23	-142.45	0.17355	57.26	-136.58
0.15970	55.28	-137.54	0.16355	56.29	-131.63
0.14970	**54.32**	**-132.65**	**0.15355**	**55.32**	**-126.68**
0.13970	53.34	-127.76	0.14355	54.32	-121.74
0.12970	52.35	-122.89	0.13355	53.31	-116.79
0.11970	51.34	-118.02	0.12355	52.28	-111.86
0.10970	50.32	-113.17	0.11355	51.23	-106.93
0.09970	49.28	-108.32	0.10355	50.17	-102.00

Propane Dew Point Calculations

The effect of changing the critical temperature on the calculated dew point for propane is shown in Table XVI (a). Increasing the critical temperature by 1 °F, increases the calculated dew point for propane by 0.77 °F for both the SRK and for the PR. Increasing the critical temperature by 5 °F, increases the dew point temperature by 3.86 °F for both the SRK and the PR. Lowering the critical temperature lowers the calculated dew point by almost the same amount.

Table XVI (a). Effect of Change in Critical Temperature on Calculated Dew Point of Propane.

Critical Temperature T (°F)	Dew Point Temperature (°F)		Enthalpy (kBTU)	
	SRK	PR	SRK	PR
211.01	58.18	59.18	559.11	560.43
210.01	57.41	58.41	557.80	559.11
209.01	56.64	57.64	556.49	557.80
208.01	55.87	56.86	555.18	556.49
207.01	55.09	56.09	553.87	555.18
206.01	**54.32**	**55.32**	**552.57**	**553.87**
205.01	53.55	54.54	551.26	552.56
204.01	52.78	53.77	549.96	551.26
203.01	52.00	52.99	548.66	549.95
202.01	51.23	52.22	547.36	548.65
201.01	50.46	51.45	546.06	547.35

Table XVII (a) shows the result of changing propane critical pressure on the calculated dew point. Results for both equations are again similar, but the changes are much smaller. An increase in critical pressure of 5 psia, decreases the calculated dew point of only 0.52 °F for the SRK and by 0.53 for the PR. Lowering the critical pressure increases the calculated dew point by almost the same amount. Increasing the critical pressure by one psi, decreases the calculated dew point calculations by 0.10 °F for the SRK and by 0.11 °F for the PR. These results are show in Table XVII (a).

Table XVII (a). Effect of Change in Critical Pressure on Calculated Dew Point of Propane.

Critical Pressure P (psia)	Dew Point Temperature (°F)		Enthalpy (kBTU)	
	SRK	PR	SRK	PR
621.35	53.80	54.79	551.94	553.24
620.35	53.91	54.90	552.06	553.37
619.35	54.01	55.00	552.19	553.49
618.35	54.11	55.11	552.31	553.62
617.35	54.22	55.21	552.44	553.74
616.35	**54.32**	**55.32**	**552.57**	**553.87**
615.35	54.43	55.42	552.69	554.00
614.35	54.53	55.53	552.82	554.13
613.35	54.63	55.63	552.95	554.25
612.35	54.74	55.74	553.07	554.38
611.35	54.85	55.84	553.20	554.51

Increasing the acentric factor from (**0.14970** to 0.15970) increases the calculated propane dew point temperature 0.96 °F for the SRK. Changing the acentric factor for the PR from (**0.15355** to 0.16355) increases the dew point temperature by 0.97 °F. The results are shown in Table XVIII (a).

Table XVIII (a). Effect of Changes in Acentric Factor on Calculated Dew Point of Propane.

Acentric Factor ω	Dew Point Temperature T (°F)	Enthalpy (kBTU)	Acentric Factor ω	Dew Point Temperature T (°F)	Enthalpy (kBTU)
SRK	SRK	SRK	PR	PR	PR
0.19970	58.99	559.82	0.20355	60.05	561.24
0.18970	58.09	558.41	0.19355	59.13	559.81
0.17970	57.17	556.99	0.18355	58.20	558.37
0.16970	56.23	555.53	0.17355	57.26	556.89
0.15970	55.28	554.06	0.16355	56.29	555.39
0.14970	**54.32**	**552.57**	**0.15355**	**55.32**	**553.87**
0.13970	53.34	551.05	0.14355	54.32	552.32
0.12970	52.35	559.51	0.13355	53.31	550.75
0.11970	51.34	547.94	0.12355	52.28	549.14
0.10970	50.32	546.35	0.11355	51.23	547.51
0.09970	49.28	544.74	0.10355	50.17	545.85

b) Binary Mixture

Bubble point, dew point and flash calculations were performed for an equimolar binary mixture of n-butane and n-pentane. The binary mixture bubble point and dew point temperature calculations were performed at 100 psia (698.48 kPa). Changes in critical temperature, critical pressure and acentric factor were made separately for each component. Tables I (b), through VI (b) show the results for bubble point calculations. Tables VII (b) through XII (b) show the results for dew point calculations. The flash calculations are performed at fixed L/F = 0.5 and at fixed pressure of 100 psia. The results for the flash calculations are presented in Tables XIII (b), XV (b), XVII (b) and XVIII (b) for n-butane and Tables XIV (b), XVI (b), XIX (b) and XX (b) for n-pentane.

Binary Mixture Bubble Point Calculations

The effect of changing the critical temperature of n-butane on the calculated bubble point for the binary mixture is shown in Table I (b). Increasing the critical temperature of n-butane by 1 °F, increases the calculated bubble point for the mixture by 0.54°F for the SRK and by 0.55 °F for the PR. Increasing the critical temperature of n-butane by 5°F, increases the bubble point temperature for the mixture by 2.71 °F for the SRK and by 2.72 °F, for the PR. Lowering the critical temperature lowers the calculated bubble point by almost the same amounts.

Table II (b) shows the result of changing n-pentane critical temperature on the calculated bubble point for the mixture. Increasing the critical temperature of n-pentane by 1 °F, increases the bubble point temperature of the mixture by 0.25 °F for the SRK and by 0.26 °F for the PR.

Increasing the critical temperature of n-pentane by 5 °F, increases the bubble point temperature of the mixture by 1.26 °F for the SRK and by 1.28 °F for the PR. Lowering the critical temperature lowers the calculated bubble point temperature by almost the same amounts.

The effect of changing the critical pressure of n-butane on the calculated bubble point for the binary mixture is shown in Table III (b). Increasing the critical pressure of n-butane by 5 psia, decreases the calculated bubble point temperature for the mixture by 0.48°F for both the SRK and the PR. Lowering the critical pressure of n-butane by 5 psia, increases the bubble point temperature for the mixture by almost the same amount. Changing the critical pressure by one psi decreases the bubble point calculation by 0.10 °F for the SRK and by 0.09 °F, for the PR.

Table IV (b) shows the result of changing n-pentane critical pressure on the calculated bubble point of the mixture. Increasing the critical pressure of n-pentane by 5 psia, decreases the bubble point temperature of the mixture by 0.28 °F for the SRK and by 0.27 °F for the PR. Changing the critical pressure by one psia decreases the bubble point of the mixture by 0.06 °F for the SRK and by 0.05 °F for the PR. Lowering the critical pressure increases the calculated bubble point by almost the same amounts.

Table I (b). Effect of Change in n-Butane Critical Temperature on Calculated Bubble Point of Equimolar Mixture of n-Butane and n-Pentane.

Critical Temperature (°F)	Bubble Point Temperature (°F)		Equilibrium Constant				Enthalpy (kBTU)	
			n-Butane (K_{C4})		n-Pentane (K_{C5})			
	SRK	PR	SRK	PR	SRK	PR	SRK	PR
310.65	179.50	180.65	1.37721	1.37300	0.62279	0.62700	282.95	292.78
309.65	178.96	180.11	1.38120	1.37696	0.61880	0.62304	281.65	291.50
308.65	178.42	179.57	1.38518	1.38091	0.61482	0.61909	280.34	290.20
307.65	177.88	179.02	1.38917	1.38486	0.61083	0.61514	279.03	288.90
306.65	177.33	178.48	1.39314	1.38881	0.60686	0.61119	277.71	287.59
305.65	**176.79**	**177.93**	**1.39712**	**1.39275**	**0.60288**	**0.60725**	**276.38**	**286.28**
304.65	176.24	177.38	1.40109	1.39669	0.59891	0.60331	275.05	284.96
303.65	175.69	176.83	1.40506	1.40063	0.59494	0.59937	273.71	283.63
302.65	175.14	176.28	1.40902	1.40457	0.59098	0.59543	272.36	282.30
301.65	174.58	175.73	1.41298	1.40849	0.58702	0.59151	271.01	280.96
300.65	174.03	175.17	1.41693	1.41242	0.58307	0.58758	269.65	279.61

Table II (b). Effect of Change in n-Pentane Critical Temperature on Calculated Bubble Point of Equimolar Mixture of n-Butane and n-pentane.

Critical Temperature (°F)	Bubble Point Temperature (°F)		Equilibrium Constant				Enthalpy (kBTU)	
			n-Butane (K_{C4})		n-Pentane (K_{C5})			
	SRK	PR	SRK	PR	SRK	PR	SRK	PR
390.79	178.05	179.21	1.41495	1.41045	0.58505	0.58955	276.09	286.12
389.79	177.80	178.96	1.41141	1.40694	0.58859	0.59306	276.16	286.17
388.79	177.55	178.70	1.40785	1.40341	0.59215	0.59659	276.23	286.20
387.79	177.30	178.45	1.40429	1.39987	0.59571	0.60013	276.29	286.23
386.79	177.04	178.19	1.40071	1.39632	0.59929	0.60369	276.34	286.26
385.79	**176.79**	**177.93**	**1.39712**	**1.39275**	**0.60288**	**0.60725**	**276.38**	**286.28**
384.79	176.53	177.67	1.39352	1.38918	0.60648	0.61082	276.42	286.29
383.79	176.27	177.41	1.38990	1.38559	0.61010	0.61441	276.46	286.30
382.79	176.01	177.15	1.38628	1.38199	0.61372	0.61801	276.48	286.30
381.79	175.75	176.89	1.38265	1.37839	0.61735	0.62162	276.51	286.29
380.79	175.48	176.62	1.37899	1.37476	0.62101	0.62524	276.52	286.28

The effect of changing the acentric factor of n-butane and n-pentane on the calculated bubble point for the binary mixture is shown in Tables V (b) and VI (b). Changing the acentric factor for n-butane from (**0.19710** to 0.20710) increases the bubble point temperature of the mixture by 0.54°F for the SRK. Changing the acentric factor for the PR from (**0.19997** to 0.20997) increases the bubble point for the mixture by 0.55 °F. These results are shown in Table V (b).

Table VI (b) shows the results of changing the acentric factor of n-pentane on the calculated bubble point temperature of the mixture. Changing the acentric factor from (**0.2490** to 0.2590) increases the bubble point by 0.40 °F for the SRK. Changing the acentric factor for the PR from (**0.24914** to 0.25914) increases the bubble point of the mixture by 0.41 °F.

Table III (b). Effect of Change in n-Butane Critical Pressure on Calculated Bubble Point of Equimolar Mixture of n-Butane and n-Pentane.

Critical Pressure (psia)	Bubble Point Temperature (°F)		Equilibrium Constant				Enthalpy (kBTU)	
			n-Butane (K_{C4})		n-Pentane (K_{C5})			
	SRK	PR	SRK	PR	SRK	PR	SRK	PR
555.65	176.31	177.45	1.40089	1.39651	0.59911	0.60349	274.34	284.26
554.65	176.40	177.54	1.40014	1.39577	0.59986	0.60423	274.75	284.66
553.65	176.50	177.64	1.39939	1.39501	0.60061	0.60499	275.16	285.06
552.65	176.60	177.74	1.39863	1.39426	0.60137	0.60574	275.56	285.47
551.65	176.69	177.84	1.39788	1.39351	0.60212	0.60649	275.97	285.87
550.65	**176.79**	**177.93**	**1.39712**	**1.39275**	**0.60288**	**0.60725**	**276.38**	**286.28**
549.65	176.88	178.03	1.39636	1.39200	0.60364	0.60800	276.80	286.68
548.65	176.98	178.13	1.39560	1.39124	0.60440	0.60876	277.21	287.09
547.65	177.08	178.23	1.39483	1.39047	0.60517	0.60953	277.62	287.50
546.65	177.17	178.32	1.39408	1.38972	0.60592	0.61028	278.03	287.91
545.65	177.27	178.42	1.39330	1.38895	0.60670	0.61105	278.45	288.32

Table IV (b). Effect of Change in n-Pentane Critical Pressure on Calculated Bubble Point of Equimolar Mixture of n-Butane and n-pentane.

Critical Pressure (psia)	Bubble Point Temperature (°F)		Equilibrium Constant				Enthalpy (kBTU)	
			n-Butane (K_{C4})		n-Pentane (K_{C5})			
	SRK	PR	SRK	PR	SRK	PR	SRK	PR
493.64	176.51	177.66	1.39405	1.38967	0.60595	0.61033	275.12	285.03
492.64	176.56	177.71	1.39466	1.39028	0.60534	0.60972	275.37	285.28
491.64	176.62	177.77	1.39527	1.39091	0.60473	0.60909	275.62	285.53
490.64	176.68	177.82	1.39589	1.39151	0.60411	0.60849	275.88	285.78
489.64	176.73	177.88	1.39650	1.39213	0.60350	0.60787	276.13	286.03
488.64	**176.79**	**177.93**	**1.39712**	**1.39275**	**0.60288**	**0.60725**	**276.38**	**286.28**
487.64	176.84	177.99	1.39773	1.39337	0.60227	0.60663	276.64	286.53
486.64	176.90	178.04	1.39835	1.39399	0.60165	0.60601	276.89	286.78
485.64	176.95	178.10	1.39897	1.39461	0.60103	0.60539	277.15	287.03
484.64	177.01	178.15	1.39959	1.39523	0.60041	0.60477	277.41	287.28
483.64	177.07	178.21	1.40021	1.39585	0.59979	0.60415	277.66	287.54

Table V (b). Effect of Changes in n-Butane Acentric Factor on Calculated Bubble Point of Equimolar Mixture of n-Butane and n-Pentane.

Acentric Factor (SRK)	Bubble Point Temperature (°F)	Equilibrium Constant		Enthalpy (kBTU)	Acentric Factor (PR)	Bubble Point Temperature T (°F)	Equilibrium Constant		Enthalpy (kBTU)
		n-Butane (K_{C4})	n-Pentane (K_{C5})				n-Butane (K_{C4})	n-Pentane (K_{C5})	
0.24710	179.41	1.37809	0.62191	268.13	0.24997	180.56	1.37382	0.62618	277.91
0.23710	178.90	1.38182	0.61818	269.81	0.23997	180.05	1.37752	0.62248	279.61
0.22710	178.39	1.38559	0.61441	271.48	0.22997	179.54	1.38126	0.61874	281.30
0.21710	177.86	1.38940	0.61060	273.13	0.21997	179.01	1.38505	0.61495	282.97
0.20710	177.33	1.39324	0.60676	274.76	0.20997	178.48	1.38888	0.61112	284.63
0.19710	**176.79**	**1.39712**	**0.60288**	**276.38**	**0.19997**	**177.93**	**1.39275**	**0.60725**	**286.28**
0.18710	176.24	1.40103	0.59897	277.99	0.18997	177.38	1.39667	0.60333	287.91
0.17710	175.68	1.40500	0.59501	279.58	0.17997	176.82	1.40062	0.59938	289.53
0.16710	175.12	1.40898	0.59102	281.15	0.16997	176.25	1.40463	0.59538	291.14
0.15710	174.55	1.41301	0.58699	282.70	0.15997	175.67	1.40867	0.59133	292.73
0.14710	173.97	1.41707	0.58293	284.24	0.14997	175.09	1.41277	0.58723	294.30

Table VI (b). Effect of Changes in n-Pentane Acentric Factor on Calculated Bubble Point of Equimolar Mixture of n-Butane and n-Pentane.

Acentric Factor (SRK)	Bubble Point Temperature (°F)	Equilibrium Constant		Enthalpy (kBTU)	Acentric Factor (PR)	Bubble Point Temperature T (°F)	Equilibrium Constant		Enthalpy (kBTU)
		n-Butane (K_{C4})	n-Pentane (K_{C5})				n-Butane (K_{C4})	n-Pentane (K_{C5})	
0.2990	178.72	1.42538	0.57462	259.11	0.29914	179.88	1.42081	0.57919	269.27
0.2890	178.35	1.41984	0.58016	262.60	0.28914	179.51	1.41533	0.58467	272.70
0.2790	177.97	1.41424	0.58576	266.07	0.27914	179.12	1.40978	0.59022	276.11
0.2690	177.58	1.40859	0.59141	269.52	0.26914	178.73	1.40417	0.59583	279.51
0.2590	177.19	1.40288	0.59712	272.96	0.25914	178.34	1.39849	0.60151	282.90
0.2490	**176.79**	**1.39712**	**0.60288**	**276.38**	0.24914	**177.93**	**1.39275**	**0.60725**	**286.28**
0.2390	176.38	1.39130	0.60870	279.79	0.23914	177.52	1.38695	0.61306	289.64
0.2290	175.97	1.38542	0.61458	283.18	0.22814	177.10	1.38107	0.61893	293.00
0.2190	175.55	1.37948	0.62052	286.55	0.21914	176.68	1.37513	0.62487	296.34
0.2090	175.13	1.37348	0.62652	289.90	0.20914	176.24	1.36912	0.63088	299.67
0.1990	174.69	1.36742	0.63258	293.23	0.19914	175.80	1.36303	0.63697	302.98

Binary Mixture Dew Point Calculations

The effect of changing the critical temperature of n-butane on the calculated dew point for the binary mixture is shown in Table VII (b). Increasing the critical temperature of n-butane by 1 °F, increases the calculated dew point for the mixture by 0.23°F for the SRK and by 0.24 °F for the PR. Increasing the critical temperature of n-butane by 5°F, increases the dew point temperature for the mixture by 1.16 °F for the SRK and by 1.18 °F, for the PR. Lowering the critical temperature lowers the calculated dew point by almost the same amounts.

Table VIII (b) shows the result of changing n-pentane critical temperature on the calculated dew point for the mixture. Increasing the critical temperature of n-pentane by 1 °F, increases the dew point temperature of the mixture by 0.56 °F for the SRK and by 0.57 °F for the PR. Increasing the critical temperature of n-pentane by 5 °F, increases the dew point temperature of the mixture by 2.83 °F for both the SRK and the PR. Lowering the critical temperature lowers the calculated dew point temperature by almost the same amounts.

The effect of changing the critical pressure of n-butane on the calculated dew point for the binary mixture is shown in Table IX (b). Increasing the critical pressure of n-butane by 5 psia, decreases the calculated dew point temperature for the mixture by 0.19 °F for the SRK and by 0.20 °F for the PR. Lowering the critical pressure of n-butane by 5 psia, increases the dew point temperature for the mixture by almost the same amount. Changing the critical pressure by one psia decreases the dew point calculation by 0.04 °F for both the SRK and the PR.

Table X (b) shows the result of changing n-pentane critical pressure on the calculated dew point of the binary mixture. Increasing the critical pressure of n-pentane by 5 psia, decreases the dew point temperature of the mixture by 0.57 °F for the SRK and by 0.56 °F for the PR. Increasing the critical pressure by one psi decreases the dew point of the mixture by 0.11 °F for both the SRK and the PR. Lowering the critical pressure increases the calculated dew point by almost the same amounts.

Table VII (b). Effect of Change in n-Butane Critical Temperature on Calculated Dew Point of Equimolar Mixture of n-Butane and n-Pentane.

Critical Temperature (°F)	Dew Point Temperature (°F)		Equilibrium Constant				Enthalpy (kBTU)	
			n-Butane (K_{C4})		n-Pentane (K_{C5})			
	SRK	PR	SRK	PR	SRK	PR	SRK	PR
310.65	193.63	194.61	1.57097	1.56244	0.73343	0.73531	1199.76	1202.09
309.65	193.40	194.37	1.57993	1.57126	0.73150	0.73337	1199.10	1201.42
308.65	193.16	194.14	1.58897	1.58016	0.72958	0.73145	1198.45	1200.75
307.65	192.93	193.90	1.59809	1.58915	0.72767	0.72954	1197.79	1200.09
306.65	192.70	193.67	1.60729	1.59821	0.72578	0.72764	1197.15	1199.43
305.65	**192.47**	**193.43**	**1.61658**	**1.60735**	**0.72390**	**0.72576**	**1196.51**	**1198.78**
304.65	192.24	193.20	1.62595	1.61658	0.72204	0.72390	1195.87	1198.14
303.65	192.01	192.97	1.63540	1.62589	0.72019	0.72205	1195.24	1197.49
302.65	191.79	192.75	1.64494	1.63528	0.71835	0.72021	1194.61	1196.86
301.65	191.56	192.52	1.65457	1.64475	0.71653	0.71839	1193.99	1196.22
300.65	191.34	192.29	1.66428	1.65431	0.71473	0.71658	1193.37	1195.60

Table VIII (b). Effect of Change in n-Pentane Critical Temperature on Calculated Dew Point of Equimolar Mixture of n-Butane and n-pentane.

Critical Temperature (°F)	Dew Point Temperature (°F)		Equilibrium Constant				Enthalpy (kBTU)	
			n-Butane (K_{C4})		n-Pentane (K_{C5})			
	SRK	PR	SRK	PR	SRK	PR	SRK	PR
390.79	195.30	196.26	1.65941	1.64952	0.71563	0.71748	1205.14	1207.40
389.79	194.73	195.70	1.65074	1.64099	0.71725	0.71911	1203.40	1205.67
388.79	194.17	195.13	1.64213	1.63251	0.71889	0.72075	1201.67	1203.94
387.79	193.60	194.56	1.63356	1.62408	0.72054	0.72240	1199.94	1202.21
386.79	193.03	194.00	1.62505	1.61569	0.72221	0.72408	1198.22	1200.50
385.79	**192.47**	**193.43**	**1.61658**	**1.60735**	**0.72390**	**0.72576**	**1196.51**	**1198.78**
384.79	191.91	192.87	1.60816	1.59906	0.72560	0.72747	1194.79	1197.07
383.79	191.34	192.31	1.59979	1.59082	0.72732	0.72919	1193.09	1195.37
382.79	190.78	191.75	1.59147	1.58262	0.72905	0.73092	1191.38	1193.67
381.79	190.22	191.19	1.58319	1.57448	0.73080	0.73267	1189.69	1191.98
380.79	189.66	190.64	1.57496	1.56637	0.73257	0.73444	1188.00	1190.29

The effect of changing the acentric factor of n-butane and n-pentane on the calculated dew point for the binary mixture is shown in Tables XI (b) and XII (b). increasing the acentric factor for n-butane from (**0.19710** to 0.20710) increases the dew point temperature of the mixture by 0.20°F for the SRK. Changing the acentric factor for the PR from (**0.19997** to 0.20997) increases the dew point for the mixture by 0.21 °F. These results are shown in Table XI (b).

Table XII (b) shows the result of changing the acentric factor of n-pentane on the calculated dew point temperature of the binary mixture. Increasing the acentric factor from (**0.2490** to 0.2590) increases the dew point by 0.82 °F for the SRK. Changing the acentric factor for the PR from (**0.24914** to 0.25914) increases the dew point of the mixture by 0.82 °F.

Table IX (b). Effect of Change in n-Butane Critical Pressure on Calculated Dew Point of Equimolar Mixture of n-Butane and n-Pentane.

Critical Pressure P (psia)	Dew Point Temperature T (°F)		Equilibrium Constant				Enthalpy (kBTU)	
			n-Butane (K_{C4})		n-Pentane (K_{C5})			
	SRK	PR	SRK	PR	SRK	PR	SRK	PR
555.65	192.28	193.23	1.62523	1.61599	0.72218	0.72402	1196.14	1198.40
554.65	192.31	193.27	1.62350	1.61426	0.72252	0.72436	1196.22	1198.48
553.65	192.35	193.31	1.62177	1.61253	0.72286	0.72471	1196.29	1198.55
552.65	192.39	193.35	1.62004	1.61080	0.72321	0.72506	1196.36	1198.63
551.65	192.43	193.39	1.61831	1.60908	0.72355	0.72541	1196.43	1198.71
550.65	**192.47**	**193.43**	**1.61658**	**1.60735**	**0.72390**	**0.72576**	**1196.51**	**1198.78**
549.65	192.51	193.47	1.61485	1.60563	0.72425	0.72612	1196.58	1198.86
548.65	192.55	193.52	1.61312	1.60391	0.72459	0.72647	1196.65	1198.93
547.65	192.59	193.56	1.61139	1.60219	0.72494	0.72682	1196.72	1199.01
546.65	192.63	193.60	1.60967	1.60046	0.72529	0.72718	1196.80	1199.09
545.65	192.66	193.64	1.60794	1.59874	0.72564	0.72753	1196.87	1199.16

Table X (b). Effect of Change in n-Pentane Critical Pressure on Calculated Dew Point of Equimolar Mixture of n-Butane and n-pentane.

Critical Pressure (psia)	Dew Point Temperature (°F)		Equilibrium Constant				Enthalpy (kBTU)	
			n-Butane (K_{C4})		n-Pentane (K_{C5})			
	SRK	PR	SRK	PR	SRK	PR	SRK	PR
493.64	191.90	192.87	1.60983	1.60056	0.72525	0.72716	1195.04	1197.33
492.64	192.02	192.98	1.61118	1.60191	0.72499	0.72688	1195.33	1197.62
491.64	192.13	193.10	1.61252	1.60326	0.72471	0.72660	1195.63	1197.91
490.64	192.24	193.21	1.61387	1.60462	0.72444	0.72632	1195.92	1198.20
489.64	192.36	193.32	1.61522	1.60598	0.72417	0.72604	1196.21	1198.49
488.64	**192.47**	**193.43**	**1.61658**	**1.60735**	**0.72390**	**0.72576**	**1196.51**	**1198.78**
487.64	192.58	193.55	1.61794	1.60873	0.72363	0.72548	1196.80	1199.07
486.64	192.70	193.66	1.61931	1.61011	0.72335	0.72520	1197.09	1199.37
485.64	192.81	193.77	1.62068	1.61149	0.72308	0.72492	1197.39	1199.66
484.64	192.93	193.89	1.62205	1.61288	0.72280	0.72464	1197.69	1199.95
483.65								

Table XI (b). Effect of Changes in n-Butane Acentric Factor on Calculated Dew Point of Equimolar Mixture of n-Butane and n-Pentane.

Acentric Factor (SRK)	Dew Point Temperature (°F)	Equilibrium Constant		Enthalpy (kBTU)	Acentric Factor (PR)	DewPoint Temperature (°F)	Equilibrium Constant		Enthalpy (kBTU)
		n-Butane (K_{C4})	n-Pentane (K_{C5})				n-Butane (K_{C4})	n-Pentane (K_{C5})	
0.24710	193.47	1.57776	0.73196	1198.77	0.24997	194.44	1.56905	0.73385	1201.09
0.23710	193.27	1.58532	0.73035	1198.32	0.23997	194.24	1.57649	0.73224	1200.63
0.22710	193.07	1.59298	0.72873	1197.86	0.22997	194.04	1.58403	0.73062	1200.17
0.21710	192.87	1.60074	0.72712	1197.41	0.21997	193.84	1.59169	0.72900	1199.71
0.20710	192.67	1.60860	0.72551	1196.96	0.20997	193.64	1.59946	0.72738	1199.24
0.19710	**192.47**	**1.61658**	**0.72390**	**1196.51**	**0.19997**	**193.43**	**1.60735**	**0.72576**	**1198.78**
0.18710	192.27	1.62466	0.72229	1196.05	0.18997	193.23	1.61536	0.72414	1198.32
0.17710	192.07	1.63285	0.72068	1195.60	0.17997	193.03	1.62349	0.72252	1197.86
0.16710	191.87	1.64116	0.71908	1195.15	0.16997	192.82	1.63175	0.72090	1197.39
0.15710	191.67	1.64958	0.71747	1194.70	0.15997	192.62	1.64013	0.71927	1196.93
0.14710	191.47	1.65811	0.71587	1194.25	0.14997	192.42	1.64863	0.71765	1196.46

Table XII (b). Effect of Changes in n-Pentane Acentric Factor on Calculated Dew Point of Equimolar Mixture of n-Butane and n-Pentane.

Acentric Factor (SRK)	Bubble Point Temperature (°F)	Equilibrium Constant		Enthalpy (kBTU)	Acentric Factor (PR)	Bubble Point Temperature (°F)	Equilibrium Constant		Enthalpy (kBTU)
		n-Butane (K_{C4})	n-Pentane (K_{C5})				n-Butane (K_{C4})	n-Pentane (K_{C5})	
0.2990	196.49	1.67943	0.71197	1208.27	0.29914	197.46	1.66922	0.71382	1210.57
0.2890	195.70	1.66688	0.71425	1205.95	0.28914	196.67	1.65691	0.71609	1208.25
0.2790	194.90	1.65432	0.71658	1203.62	0.27914	195.87	1.64456	0.71842	1205.91
0.2690	194.10	1.64175	0.71896	1201.26	0.26914	195.07	1.63219	0.72081	1203.56
0.2590	193.29	1.62917	0.72140	1198.89	0.25914	194.25	1.61978	0.72326	1201.18
0.2490	**192.47**	**1.61658**	**0.72390**	**1196.51**	**0.24914**	**193.43**	**1.60735**	**0.72576**	**1198.78**
0.2390	191.65	1.60398	0.72645	1194.10	0.23914	192.61	1.59489	0.72833	1196.36
0.2290	190.82	1.59139	0.72907	1191.68	0.22814	191.77	1.58241]	0.73097	1193.93
0.2190	189.98	1.57879	0.73174	1189.25	0.21914	190.93	1.56991	0.73367	1191.47
0.2090	189.14	1.56618	0.73448	1186.79	0.20914	190.08	1.55738	0.73643	1188.99
0.1990	188.29	1.55358	0.73729	1184.33	0.19914				

Binary Mixture Flash Calculations

The effect of changing the critical temperature of n-butane on the calculated temperature to obtain 50% (mole) vapor and 50% (mole) liquid for the binary mixture is shown in Table XIII (b). Increasing the critical temperature of n-butane by 1 °F, increases the required flash temperature by 0.38 °F for both the SRK and the PR. Increasing the critical temperature by 5 °F, increases the required flash temperature by 1.91 °F for both the SRK and the PR. Lowering the critical temperature lowers the calculated flash temperature by almost the same amounts.

The effect of changing the critical temperature of n-pentane on the calculated flash temperature for the binary mixture is shown in Table XIV (b). Increasing the critical temperature of n-pentane by 1 °F, increases the calculated flash temperature by 0.40 °F for both the SRK and the PR. Increasing the critical temperature of n-pentane by 5 °F, increases the calculated flash temperature by about 2.10 °F for both the SRK and the PR. Lowering the critical temperature lowers the calculated flash temperature by almost the same amounts.

Table XV (b) shows the effect of changing the critical pressure of n-butane on the calculated flash temperature for the binary mixture. Increasing the critical pressure of n-butane by 5 psia, decreases the calculated flash temperature for the mixture by about 0.30°F for both the SRK and °F the PR. Lowering the critical pressure of n-butane by 5 psia, increases the flash temperature for the mixture by almost the same amount. Increasing the critical pressure of by one psia decreases the flash temperature calculation by 0.07 °F for both the SRK and the PR.

Table XIII (b). Effect of Change in n-Butane Critical Temperature on Flash Calculations at fixed P and L/F=0.5 of Equimolar Mixture of n-Butane and n-Pentane.

Critical Temperature (°F)	Liquid Mole Fraction				Flash Temperature (°F)		Equilibrium Constant				Enthalpy (kBTU)	
	n-Butane		n-Pentane				n-Butane		n- Pentane			
	SRK	PR	SRK	PR	SRK	PR	SRK	PR	SRK	PR	SRK	PR
310.65	0.4041	0.4051	0.5959	0.5949	186.74	187.79	1.47490	1.46838	0.67801	0.68101	737.12	743.29
309.65	0.4030	0.4041	0.5970	0.5959	186.36	187.41	1.48141	1.47481	0.67503	0.67806	736.06	742.23
308.65	0.4019	0.4030	0.5981	0.5970	185.98	187.02	1.48795	1.48126	0.67206	0.67510	734.99	741.16
307.65	0.4009	0.4020	0.5991	0.5980	185.60	186.64	1.49453	1.48775	0.66910	0.67215	733.92	740.10
306.65	0.3998	0.4009	0.6002	0.5991	185.22	186.26	1.50116	1.49429	0.66615	0.66921	732.85	739.03
305.65	**0.3988**	**0.3999**	**0.6012**	**0.6001**	**184.84**	**185.88**	**1.50782**	**1.50087**	**0.66321**	**0.66629**	**731.78**	**737.96**
304.65	0.3977	0.3988	0.6023	0.6012	184.45	185.49	1.51453	1.50747	0.66027	0.66336	730.70	736.89
303.65	0.3966	0.3978	0.6034	0.6022	184.07	185.11	1.52128	1.51413	0.65734	0.66045	729.63	735.82
302.65	0.3956	0.3967	0.6044	0.6033	183.69	184.73	1.52807	1.52082	0.65442	0.65754	728.55	734.74
301.65	0.3945	0.3956	0.6055	0.6044	183.31	184.35	1.53490	1.52755	0.65151	0.65464	727.48	733.67
300.65	0.3934	0.3946	0.6066	0.6054	182.93	183.97	1.54177	1.53433	0.64860	0.65175	726.40	732.59

Table XIV (b). Effect of Change in n-Pentane Critical Temperature on Flash Calculations at fixed P and L/F=0.5 of Equimolar Mixture of n-Butane and n-Pentane.

Critical Temperature (°F)	Liquid Mole Fraction				Flash Temperature (°F)		Equilibrium Constant				Enthalpy (kBTU)	
	n-Butane		n-Pentane				n-Butane		n-Pentane			
	SRK	PR	SRK	PR	SRK	PR	SRK	PR	SRK	PR	SRK	PR
390.79	0.3940	0.3951	0.6060	0.6049	186.92	187.97	1.53833	1.53093	0.65006	0.65320	735.52	741.77
389.79	0.3949	0.3961	0.6051	0.6039	186.51	187.55	1.53219	1.52488	0.65266	0.65579	734.78	741.01
388.79	0.3959	0.3970	0.6041	0.6030	186.09	187.13	1.52607	1.51885	0.65528	0.65839	734.03	740.25
387.79	0.3968	0.3980	0.6032	0.6020	185.67	186.71	1.51997	1.51283	0.65791	0.66101	733.28	739.49
386.79	0.3978	0.3989	0.6022	0.6011	185.25	186.29	1.51389	1.50684	0.66055	0.66364	732.53	738.72
385.79	**0.3988**	**0.3999**	**0.6012**	**0.6001**	**184.84**	**185.88**	**1.50782**	**1.50087**	**0.66321**	**0.66629**	**731.78**	**737.96**
384.79	0.3997	0.4008	0.6003	0.5992	184.42	185.46	1.50178	1.49490	0.66587	0.66894	731.02	737.19
383.79	0.4007	0.4018	0.5993	0.5982	184.00	185.04	1.49576	1.48896	0.66856	0.67161	730.27	736.43
382.79	0.4016	0.4027	0.5984	0.5973	183.58	184.62	1.48975	1.48304	0.67125	0.67429	729.52	735.66
381.79	0.4026	0.4037	0.5974	0.5963	183.16	184.21	1.48377	1.47714	0.67396	0.67698	728.76	734.89
380.79	0.4036	0.4047	0.5964	0.5953	182.75	183.79	1.47780	1.47126	0.67668	0.67969	728.01	734.12

Table XVI (b) shows the result of changing n-pentane critical pressure on the required flash temperature of the mixture. Increasing the critical pressure of n-pentane by 5 psia, decreases the required flash temperature by 0.43 °F for both the SRK and the PR. Increasing the critical pressure by one psia decreases the required flash temperature of the mixture by 0.09 °F for both the SRK and the PR. Lowering the critical pressure increases the calculated flash temperature by almost the same amounts.

The effect of changing the acentric factor of n-butane and n-pentane on the calculated flash temperature for the binary mixture is shown in Tables XVII (b) and XVIII (b). increasing the acentric factor for n-butane from (**0.19710** to 0.20710) increases the required flash temperature of the mixture by 0.35°F for the SRK. increasing the acentric factor for the PR from (**0.19997** to 0.20997) increases the required flash temperature by 0.05 °F. These results are shown in Table XVII (b).

Table XIX (b) shows the result of changing the acentric factor of n-pentane on the calculated flash temperature of the mixture. Changing the acentric factor from (**0.2490** to 0.2590) increases the flash temperature by about 0.60 °F for the SRK. increasing the acentric factor for the PR from (**0.24914** to 0.25914) increases the flash temperature of the mixture by about 0.60 °F.

Table XV (b). Effect of Change in n-Butane Critical Pressure on Flash Calculations at fixed P and L/F=0.5 of Equimolar Mixture of n-Butane and n-Pentane.

Critical Pressure (psia)	Liquid Mole Fraction				Flash Temperature (°F)		Equilibrium Constant				Enthalpy (kBTU)	
	n-Butane		n-Pentane				n-Butane		n-Pentane			
	SRK	PR	SRK	PR	SRK	PR	SRK	PR	SRK	PR	SRK	PR
555.65	0.3978	0.3989	0.6022	0.6011	184.51	185.54	1.51410	1.50711	0.66046	0.66352	730.61	736.79
554.65	0.3980	0.3991	0.6020	0.6009	184.57	185.61	1.51285	1.50586	0.66100	0.66407	730.84	737.02
553.65	0.3982	0.3993	0.6018	0.6007	184.64	185.68	1.51159	1.50461	0.66155	0.66462	731.07	737.25
552.65	0.3984	0.3995	0.6016	0.6005	184.70	185.74	1.51034	1.50336	0.66210	0.66518	731.31	737.49
551.65	0.3986	0.3997	0.6014	0.6003	184.77	185.81	1.50908	1.50211	0.66265	0.66573	731.54	737.72
550.65	**0.3988**	**0.3999**	**0.6012**	**0.6001**	**184.84**	**185.88**	**1.50782**	**1.50087**	**0.66321**	**0.66629**	**731.78**	**737.96**
549.65	0.3990	0.4001	0.6010	0.5999	184.90	185.94	1.50657	1.49961	0.66376	0.66684	732.01	738.19
548.65	0.3992	0.4003	0.6008	0.5997	184.97	186.01	1.50531	1.49836	0.66431	0.66740	732.25	738.43
547.65	0.3994	0.4005	0.6006	0.5995	185.03	186.08	1.50405	1.49711	0.66487	0.66795	732.48	738.67
546.65	0.3996	0.4007	0.6004	0.5993	185.10	186.15	1.50279	1.49586	0.66543	0.66851	732.72	738.90
545.65	0.3998	0.4009	0.6002	0.5991	185.17	186.21	1.50153	1.49461	0.66598	0.66907	732.96	739.14

Table XVI (b). Effect of Change in n-Pentane Critical Pressure on Flash Calculations at fixed P and L/F=0.5 of Equimolar Mixture of n-Butane and n-Pentane.

Critical Pressure (psia)	Liquid Mole Fraction				Flash Temperature (°F)		Equilibrium Constant				Enthalpy (kBTU)	
	n-Butane		n-Pentane				n-Butane		n-Pentane			
	SRK	PR	SRK	PR	SRK	PR	SRK	PR	SRK	PR	SRK	PR
493.64	0.3995	0.4007	0.6005	0.5993	184.41	185.45	1.50284	1.49586	0.66541	0.66851	730.34	736.54
492.64	0.3994	0.4005	0.6006	0.5995	184.49	185.54	1.50383	1.49685	0.66497	0.66807	730.63	736.83
491.64	0.3992	0.4003	0.6008	0.5997	184.58	185.62	1.50483	1.49785	0.66453	0.66762	730.91	737.11
490.64	0.3991	0.4002	0.6009	0.5998	184.66	185.71	1.50582	1.49885	0.66409	0.66718	731.20	737.39
489.64	0.3989	0.4000	0.6011	0.6000	184.75	185.79	1.50682	1.49986	0.66365	0.66673	731.49	737.67
488.64	**0.3988**	**0.3999**	**0.6012**	**0.6001**	**184.84**	**185.88**	**1.50782**	**1.50087**	**0.66321**	**0.66629**	**731.78**	**737.96**
487.64	0.3986	0.3997	0.6014	0.6003	184.92	185.96	1.50883	1.50187	0.66277	0.66583	732.07	738.24
486.64	0.3984	0.3995	0.6016	0.6005	185.01	186.05	1.50984	1.50289	0.66232	0.66539	732.36	738.53
485.64	0.3983	0.3994	0.6017	0.6006	185.09	186.13	1.51085	1.50390	0.66188	0.66494	732.65	738.82
484.64	0.3981	0.3992	0.6019	0.6008	185.18	186.22	1.51186	1.50492	0.66143	0.66449	732.94	739.10
483.64	0.3979	0.3991	0.6021	0.6009	185.27	186.31	1.51288	1.50594	0.66099	0.66404	733.23	739.39

Table XVII (b). Effect of Changes in n-Butane-Acentric Factor on Flash Calculations at fixed P and L/F=0.5 of Equimolar Mixture of n-Butane and n-Pentane (SRK).

Acentric Factor	Liquid Mole Fraction		Flash Temperature (°F)	Equilibrium Constant		Enthalpy (kBTU)
	n-Butane	n-Pentane		n-Butane	n-Pentane	
0.24710	0.4035	0.5965	186.57	1.47811	0.67654	730.48
0.23710	0.4026	0.5974	186.23	1.48390	0.67390	730.76
0.22710	0.4016	0.5984	185.88	1.48976	0.67125	731.03
0.21710	0.4007	0.5993	185.54	1.49570	0.66858	731.29
0.20710	0.3997	0.6003	185.19	1.50172	0.66590	731.54
0.19710	**0.3988**	**0.6012**	**184.84**	**1.50782**	**0.66321**	**731.78**
0.18710	0.3978	0.6022	184.48	1.51401	0.66050	732.00
0.17710	0.3968	0.6032	184.12	1.52029	0.65777	732.21
0.16710	0.3958	0.6042	183.76	1.52665	0.65503	732.40
0.15710	0.3948	0.6052	183.39	1.53310	0.65227	732.58
0.14710	0.3938	0.6062	183.03	1.53964	0.64950	732.75

Table XVIII (b). Effect of Changes in n-Butane Acentric Factor on Flash Calculations at fixed P and L/F=0.5 of Equimolar Mixture of n-Butane and n-Pentane (PR).

Acentric Factor	Liquid Mole Fraction		Flash Temperature (°F)	Equilibrium Constant		Enthalpy (kBTU)
	n-Butane	n-Pentane		n-Butane	n-Pentane	
0.24997	0.4046	0.5954	187.62	1.47149	0.67958	736.62
0.23997	0.4037	0.5963	187.28	1.47719	0.67696	736.91
0.22997	0.4027	0.5973	186.93	1.48298	0.67432	737.19
0.21997	0.4018	0.5982	186.59	1.48885	0.67166	737.46
0.20997	0.4008	0.5992	186.23	1.49481	0.66898	737.72
0.19997	**0.3999**	**0.6001**	**185.88**	**1.50087**	**0.66629**	**737.96**
0.18997	0.3989	0.6011	185.52	1.50701	0.66357	738.19
0.17997	0.3979	0.6021	185.16	1.51325	0.66083	738.41
0.16997	0.3969	0.6031	184.79	1.51958	0.65808	738.61
0.15997	0.3959	0.6041	184.42	1.52601	0.65530	738.81
0.14997	0.3949	0.6051	184.04	1.53255	0.65251	738.98

Table XIX (b). Effect of Changes in n-Pentane-Acentric Factor on Flash Calculations at fixed P and L/F=0.5 of Equimolar Mixture of n-Butane and n-Pentane (SRK).

Acentric Factor	Liquid Mole Fraction		Flash Temperature (°F)	Equilibrium Constant		Enthalpy (kBTU)
	n-Butane	n-Pentane		n-Butane	n-Pentane	
0.2990	0.3915	0.6085	187.92	1.55447	0.64331	726.99
0.2890	0.3929	0.6071	187.31	1.54518	0.64717	727.99
0.2790	0.3943	0.6057	186.70	1.53587	0.65110	728.97
0.2690	0.3958	0.6042	186.09	1.52654	0.65508	729.93
0.2590	0.3973	0.6027	185.46	1.51719	0.65911	730.86
0.2490	**0.3988**	**0.6012**	**184.84**	**1.50782**	**0.66321**	**731.78**
0.2390	0.4003	0.5997	184.20	1.49844	0.66736	732.67
0.2290	0.4018	0.5982	183.56	1.48903	0.67158	733.53
0.2190	0.4033	0.5967	182.92	1.47961	0.67586	734.37
0.2090	0.4048	0.5952	182.27	1.47016	0.68020	735.19
0.1990	0.4064	0.5936	181.61	1.46069	0.68460	735.98

Table XX (b). Effect of Changes in n-Pentane Acentric Factor on Flash Calculations at fixed P and L/F=0.5 of Equimolar Mixture of n-Butane and n-Pentane (PR).

Acentric Factor	Liquid Mole Fraction		Flash Temperature (°F)	Equilibrium Constant		Enthalpy (kBTU)
	n-Butane	n-Pentane		n-Butane	n-Pentane	
0.29914	0.3926	0.6074	188.97	1.54686	0.64647	733.34
0.28914	0.3941	0.6059	188.36	1.53773	0.65031	734.30
0.27914	0.3955	0.6045	187.75	1.52856	0.65421	735.25
0.26914	0.3969	0.6031	187.13	1.51936	0.65817	736.17
0.25914	0.3984	0.6016	186.51	1.51013	0.66219	737.08
0.24914	**0.3999**	**0.6001**	**185.88**	**1.50087**	**0.66629**	**737.96**
0.23914	0.4014	0.5986	185.24	1.49156	0.67044	738.82
0.22914	0.4029	0.5971	184.59	1.48222	0.67466	739.66
0.21914	0.4044	0.5956	183.94	1.47286	0.67896	740.47
0.20914	0.4059	0.5941	183.29	1.46345	0.68332	741.26
0.19914	0.4075	0.5925	182.62	1.45401	0.68775	742.03

c) Muticomponent Mixture

Flash calculations were performed at 100 psia and 100 °F for a multicom-ponent hydrocarbon mixture with components ranging from methane to n-heptane. Calculations were carried out to see how changes in pure component properties influenced the calculation results. Arbitrary changes in critical temperature, critical pressure and acentric factor were made for methane, ethane, n-butane and n-heptane. A sample of the computer output for one flash calculation is shown in Appendix A. The result summaries for the flash calculations are presented in Tables I (c) through XXIV (c). These results show that phase behavior predictions depend on the pure component properties that have been used. The predicted equilibrium constants changed because of the changes made in these properties. The change in the equilibrium constant is more noticeable for the compound for which properties were changed.

Table I (c). Effect of Change in Methane Critical Temperature on Flash Calculation at fixed P and T of a Gas Mixture (SRK).

Critical Temperature (°F)	FLASH CALCULATION EQUILIBRIUM CONSTANT							Enthalpy (KBTU)
	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}	SRK
-111.63	26.67336	5.61081	1.73929	0.53990	0.17551	0.05882	0.01996	497.78
-112.63	26.87784	5.61067	1.73908	0.53979	0.17546	0.05880	0.01995	497.82
-113.63	27.08378	5.61053	1.73888	0.53967	0.17540	0.05877	0.01994	497.85
-114.63	27.29123	5.61039	1.73867	0.53956	0.17535	0.05875	0.01993	497.89
-115.63	27.50012	5.61025	1.73846	0.53944	0.17530	0.05873	0.01992	497.92
-116.63	**27.71049**	**5.61010**	**1.73825**	**0.53933**	**0.17524**	**0.05870**	**0.01991**	**497.96**
-117.63	27.92238	5.60995	1.73804	0.53921	0.17519	0.05868	0.01990	497.99
-118.63	28.13577	5.60980	1.73783	0.53909	0.17514	0.05866	0.01989	498.02
-119.63	28.35066	5.60964	1.73761	0.53898	0.17508	0.05863	0.01988	498.06
-120.63	28.56710	5.60948	1.73740	0.53886	0.17503	0.05861	0.01987	498.09

Table II (c). Effect of Change in Methane Critical Temperature on Flash Calculation at fixed P and T of a Gas Mixture (PR).

Critical Temperature (°F)	FLASH CALCULATION EQUILIBRIUM CONSTANT							Enthalpy (KBTU)
	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}	PR
-111.63	26.38862	5.53893	1.71560	0.53646	0.17739	0.05997	0.02082	498.46
-112.63	26.59308	5.53880	1.71540	0.53634	0.17733	0.05995	0.02081	498.50
-113.63	26.79909	5.53867	1.71519	0.53623	0.17728	0.05993	0.02080	498.53
-114.63	27.00654	5.53853	1.71499	0.53611	0.17722	0.05990	0.02079	498.57
-115.63	27.21553	5.53840	1.71478	0.53599	0.17717	0.05988	0.02078	498.60
-116.63	**27.42606**	**5.53826**	**1.71457**	**0.53588**	**0.17711**	**0.059986**	**0.02077**	**498.64**
-117.63	27.63810	5.53811	1.71437	0.53576	0.17706	0.05983	0.02076	498.67
-118.63	27.85170	5.53797	1.71416	0.53565	0.17701	0.05981	0.02075	498.71
-119.63	28.06684	5.53781	1.71395	0.53553	0.17695	0.05978	0.02074	498.74
-120.63	28.28355	5.53766	1.71374	0.53542	0.17690	0.05976	0.02073	498.78

Table III (c). Effect of Change in Methane Critical Pressure on Flash Calculation at fixed P and T of a Gas Mixture (SRK).

Critical Pressure (psia)	FLASH CALCULATION EQUILIBRIUM CONSTANT							Enthalpy (KBTU)
	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}	SRK
672.75	27.72128	5.60996	1.73805	0.53922	0.17519	0.05868	0.01990	497.98
671.75	27.71905	5.60999	1.73809	0.53924	0.17520	0.05869	0.01990	497.97
670.75	27.71686	5.61002	1.73813	0.53926	0.17521	0.05869	0.01991	497.97
669.75	27.71471	5.61005	1.73817	0.53928	0.17522	0.05869	0.01991	497.96
668.75	27.71258	5.61007	1.73821	0.53930	0.17523	0.05870	0.01991	497.96
667.75	**27.71049**	**5.61010**	**1.73825**	**0.53933**	**0.17524**	**0.05870**	**0.01991**	**497.96**
666.75	27.70847	5.61013	1.73829	0.53935	0.17525	0.05871	0.01991	497.95
665.75	27.70646	5.61016	1.73833	0.53937	0.17526	0.05871	0.01991	497.95
664.75	27.70451	5.61019	1.73837	0.53939	0.17527	0.05872	0.01992	497.94
663.75	27.70260	5.61022	1.73841	0.53941	0.17528	0.05872	0.01992	497.94

Table IV (c). Effect of Change in Methane Critical Pressure on Flash Calculation at fixed P and T of a Gas Mixture (PR).

Critical Pressure (psia)	FLASH CALCULATION EQUILIBRIUM CONSTANT							Enthalpy (KBTU)
	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}	PR
672.75	27.45220	5.53809	1.71436	0.53576	0.17706	0.05983	0.02076	498.67
671.75	27.44690	5.53812	1.71440	0.53579	0.17707	0.05984	0.02077	498.66
670.75	27.44164	5.53815	1.71445	0.53581	0.17708	0.05984	0.02077	498.66
669.75	27.43640	5.53819	1.71449	0.53583	0.17709	0.05985	0.02077	498.65
668.75	27.43120	5.53822	1.71453	0.53586	0.17710	0.05985	0.02077	498.64
667.75	**27.42606**	**5.53826**	**1.71457**	**0.53588**	**0.17711**	**0.05986**	**0.02077**	**498.64**
666.75	27.42093	5.53829	1.71461	0.53590	0.17712	0.05986	0.02078	498.63
665.75	27.41582	5.53832	1.71466	0.53593	0.17714	0.05987	0.02078	498.63
664.75	27.41078	5.53836	1.71470	0.53595	0.17715	0.05987	0.02078	498.62
663.75	27.40574	5.53839	1.71474	0.53597	0.17716	0.05987	0.02078	498.62

Table V (c). Effect of Change in Methane Acentric Factor on Flash Calculation at fixed P and T of a Gas Mixture (SRK).

Acentric Factor (SRK)	FLASH CALCULATION EQUILIBRIUM CONSTANT							Enthalpy (KBTU)
	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}	SRK
0.00890	27.91968	5.61000	1.73811	0.53925	0.17521	0.05869	0.01990	497.95
0.00790	27.87774	5.61003	1.73814	0.53927	0.17522	0.05869	0.01991	497.95
0.00690	27.83584	5.61004	1.73817	0.53928	0.17522	0.05869	0.01991	497.95
0.00590	27.79402	5.61006	1.73820	0.53930	0.17523	0.05870	0.01991	497.95
0.00490	27.75223	5.61008	1.73822	0.53931	0.17524	0.05870	0.01991	497.96
0.00390	**27.71049**	**5.61010**	**1.73825**	**0.53932**	**0.17524**	**0.05870**	**0.01991**	**497.96**
0.00290	27.66884	5.61012	1.73828	0.53934	0.17525	0.05871	0.01991	497.96
0.00190	27.62722	5.61014	1.73830	0.53935	0.17526	0.05871	0.01991	497.96
0.00090	27.58566	5.61016	1.73833	0.53937	0.17526	0.05871	0.01991	497.96
0.00010	27.55243	5.61017	1.73835	0.53938	0.17527	0.05871	0.01992	497.96

Table VI (c). Effect of Change in Methane Acentric Factor on Flash Calculation at fixed P and T of a Gas Mixture (PR).

Acentric Factor (PR)	FLASH CALCULATION EQUILIBRIUM CONSTANT							Enthalpy (KBTU)
	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}	PR
0.06400	29.59413	5.53740	1.71326	0.53514	0.17677	0.05970	0.02071	498.63
0.05400	29.15025	5.53758	1.71352	0.53529	0.17684	0.05973	0.02072	498.63
0.04400	28.71156	5.53776	1.71379	0.53544	0.17691	0.05976	0.02074	498.63
0.03400	28.27798	5.53793	1.71405	0.53558	0.17697	0.05979	0.02075	498.63
0.02400	27.84948	5.53809	1.71431	0.53573	0.17704	0.05983	0.02076	498.64
0.01400	**27.42606**	**5.53826**	**1.71457**	**0.53588**	**0.17711**	**0.05986**	**0.02077**	**498.64**
0.00400	27.00766	5.53841	1.71483	0.53603	0.17718	0.05989	0.02079	498.64
0.00300	26.96610	5.53843	1.71486	0.53604	0.17719	0.05989	0.02079	498.64
0.00200	26.92458	5.53844	1.71489	0.53606	0.17720	0.05989	0.02079	498.64
0.00100	26.88311	5.53846	1.71491	0.53607	0.17721	0.05990	0.02079	498.64

Table VII (c). Effect of Change in Ethane Critical Temperature on Flash Calculation at fixed P and T of a Gas Mixture (SRK).

Critical Temperature (°F)	FLASH CALCULATION EQUILIBRIUM CONSTANT							Enthalpy (KBTU)
	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}	SRK
95.09	27.70789	5.37028	1.73835	0.53939	0.17528	0.05872	0.01992	497.91
94.09	27.70841	5.41744	1.73833	0.53938	0.17527	0.05871	0.01992	497.92
93.09	27.70896	5.46499	1.73831	0.53936	0.17526	0.05871	0.01991	497.93
92.09	27.7046	5.51296	1.73829	0.53935	0.17526	0.05871	0.01991	497.94
91.09	27.70998	5.56132	1.73827	0.53934	0.17525	0.05871	0.01991	497.95
90.09	**27.71049**	**5.61010**	**1.73825**	**0.53933**	**0.17524**	**0.05870**	**0.01991**	**497.96**
89.09	27.71104	5.65929	1.73823	0.53931	0.17524	0.05870	0.01991	497.96
88.09	27.71156	5.70890	1.73821	0.53930	0.17523	0.05870	0.01991	497.97
87.09	27.71207	5.75892	1.73819	0.53929	0.17522	0.05869	0.01991	497.98
86.09	27.71259	5.80938	1.73817	0.53927	0.17522	0.05869	0.01991	497.99

Table VIII (c). Effect of Change in Ethane Critical Temperature on Flash Calculation at fixed P and T of a Gas Mixture (PR).

Critical Temperature (°F)	FLASH CALCULATION EQUILIBRIUM CONSTANT							Enthalpy (KBTU)
	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}	PR
95.09	27.42341	5.30249	1.71466	0.53594	0.17715	0.05987	0.02078	498.60
94.09	27.42395	5.34885	1.71465	0.53593	0.17714	0.05987	0.02078	498.60
93.09	27.42448	5.39560	1.71463	0.53592	0.17713	0.05986	0.02078	498.61
92.09	27.42499	5.44275	1.71461	0.53590	0.17713	0.05986	0.02078	498.62
91.09	27.42552	5.49030	1.71459	0.53589	0.17712	0.05986	0.02078	498.63
90.09	**27.42606**	**5.53826**	**1.71457**	**0.53588**	**0.17711**	**0.05986**	**0.02077**	**498.64**
89.09	27.71104	5.65929	1.73823	0.53931	0.17524	0.05870	0.01991	497.96
88.09	27.42710	5.63538	1.71453	0.53585	0.17710	0.05985	0.02077	498.66
87.09	27.42762	5.68456	1.71452	0.53584	0.17710	0.05985	0.02077	498.67
86.09	27.42815	5.73416	1.71450	0.53583	0.17709	0.05984	0.02077	498.67

Table IX (c). Effect of Change in Ethane Critical Pressure on Flash Calculation at fixed P and T of a Gas Mixture (SRK).

Critical Pressure (psia)	FLASH CALCULATION EQUILIBRIUM CONSTANT							Enthalpy (KBTU)
	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}	SRK
712.78	27.71192	5.62876	1.73823	0.53931	0.17523	0.05870	0.01991	497.96
711.78	27.71165	5.62502	1.73824	0.53931	0.17524	0.05870	0.01991	497.96
710.78	27.71137	5.62127	1.73824	0.53931	0.17524	0.05870	0.01991	497.96
709.78	27.71106	5.61754	1.73824	0.53932	0.17524	0.05870	0.01991	497.96
708.78	27.71079	5.61382	1.73825	0.53932	0.17524	0.05870	0.01991	497.96
707.78	**27.71049**	**5.61010**	**1.73825**	**0.53933**	**0.17524**	**0.05870**	**0.01991**	**497.96**
706.78	27.71020	5.60639	1.73825	0.53933	0.17525	0.05870	0.01991	497.95
705.78	27.70994	5.60268	1.73826	0.53933	0.17525	0.05870	0.01991	497.95
704.78	27.70964	5.59899	1.73826	0.53934	0.17525	0.05871	0.01991	497.95
703.78	27.70934	5.59529	1.73826	0.53934	0.17525	0.05871	0.01991	497.95

Table X (c). Effect of Change in Ethane Critical Pressure on Flash Calculation at fixed P and T of a Gas Mixture (PR).

Critical Pressure (psia)	FLASH CALCULATION EQUILIBRIUM CONSTANT							Enthalpy (KBTU)
	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}	PR
712.78	27.42741	5.55931	1.71455	0.53586	0.17710	0.05985	0.02077	498.65
711.78	27.42713	5.55508	1.71455	0.53586	0.17711	0.05985	0.02077	498.65
710.78	27.42686	5.55087	1.71456	0.53587	0.17711	0.05985	0.02077	498.64
709.78	27.42660	5.54666	1.71457	0.53587	0.17711	0.05985	0.02077	498.64
708.78	27.42632	5.54245	1.71457	0.53588	0.17711	0.05985	0.02077	498.64
707.78	**27.42606**	**5.53826**	**1.71457**	**0.53588**	**0.17711**	**0.05986**	**0.02077**	**498.64**
706.78	27.42578	5.53406	1.71458	0.53588	0.17712	0.05986	0.02077	498.64
705.78	27.42550	5.52988	1.71458	0.53589	0.17712	0.05986	0.02077	498.64
704.78	27.42522	5.52570	1.71458	0.53589	0.17712	0.05986	0.02078	498.63
703.78	27.42495	5.52153	1.71459	0.53589	0.17712	0.05986	0.02078	498.63

Table XI (c). Effect of Change in Ethane Acentric Factor on Flash Calculation at fixed P and T of a Gas Mixture (SRK).

Acentric Factor (SRK)	FLASH CALCULATION EQUILIBRIUM CONSTANT							Enthalpy (KBTU)
	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}	SRK
0.14440	27.71057	5.63067	1.73824	0.53932	0.17524	0.05870	0.01991	497.92
0.13440	27.71055	5.62657	1.73824	0.53932	0.17524	0.05870	0.01991	497.93
0.12440	27.71054	5.62246	1.73824	0.53932	0.17524	0.05870	0.01991	497.94
0.11440	27.71053	5.61835	1.73825	0.53932	0.17524	0.05870	0.01991	497.94
0.10440	27.71051	5.61423	1.73825	0.53932	0.17524	0.05870	0.01991	497.95
0.09440	**27.71049**	**5.61010**	**1.73825**	**0.53932**	**0.17524**	**0.05870**	**0.01991**	**497.96**
0.08440	27.71048	5.60597	1.73825	0.53933	0.17524	0.05870	0.01991	497.96
0.07440	27.71047	5.60183	1.73825	0.53933	0.17524	0.05870	0.01991	497.97
0.06440	27.71044	5.59768	1.73825	0.53933	0.17524	0.05870	0.01991	497.97
0.05440	27.71044	5.59353	1.73825	0.53933	0.17524	0.05870	0.01991	497.98

Table XII (c). Effect of Change in Ethane Acentric Factor on Flash Calculation at fixed P and T of a Gas Mixture (PR).

Acentric Factor (PR)	FLASH CALCULATION EQUILIBRIUM CONSTANT							Enthalpy (KBTU)
	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}	PR
0.14947	27.42612	5.55869	1.71457	0.53588	0.17711	0.05986	0.02077	498.61
0.13947	27.42612	5.55463	1.71457	0.53588	0.17711	0.05986	0.02077	498.61
0.12947	27.42611	5.55055	1.71457	0.53588	0.17711	0.05986	0.02077	498.62
0.11947	27.42609	5.54646	1.71457	0.53588	0.17711	0.05986	0.02077	498.63
0.10947	27.42607	5.54237	1.71457	0.53588	0.17711	0.05986	0.02077	498.63
0.09947	**27.42606**	**5.53826**	**1.71457**	**0.53588**	**0.17711**	**0.05986**	**0.02077**	**498.64**
0.08947	27.42605	5.53414	1.71457	0.53588	0.17711	0.05986	0.02077	498.65
0.07947	27.42603	5.53000	1.71458	0.53588	0.17712	0.05986	0.02077	498.65
0.06947	27.42600	5.52585	1.71458	0.53588	0.17712	0.5986	0.02077	498.66
0.05947	27.42597	5.52169	1.71458	0.53588	0.17712	0.05986	0.02077	498.67

Table XIII (c). Effect of Change in n-Butane Critical Temperature on Flash Calculation at fixed P and T of a Gas Mixture (SRK).

Critical Temperature (°F)	FLASH CALCULATION EQUILIBRIUM CONSTANT							Enthalpy (KBTU)
	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}	SRK
310.65	27.71211	5.61032	1.73831	0.51095	0.17525	0.05871	0.01991	497.85
309.65	27.71174	5.61027	1.73830	0.51651	0.17525	0.05871	0.01991	497.87
308.65	27.71140	5.61022	1.73829	0.52212	0.17625	0.05870	0.01991	497.89
307.65	27.71107	5.61018	1.73827	0.52780	0.17525	0.05870	0.01991	497.91
306.65	27.71078	5.61014	1.73826	0.53353	0.17525	0.05870	0.01991	497.93
305.65	**27.71049**	**5.61010**	**1.73825**	**0.53933**	**0.17524**	**0.05870**	**0.01991**	**497.96**
304.65	27.71023	5.61006	1.73824	0.54518	0.17524	0.05870	0.01991	497.98
303.65	27.70999	5.61003	1.73822	0.55110	0.17524	0.05870	0.01991	498.00
302.65	27.70977	5.60999	1.73821	0.55708	0.17524	0.05870	0.01991	498.02
301.65	27.70928	5.60997	1.73820	0.56313	0.17524	0.05870	0.01991	498.04

Table XIV (c). Effect of Change in n-Butane Critical Temperature on Flash Calculation at fixed P and T of a Gas Mixture (PR).

Critical Temperature (°F)	FLASH CALCULATIONS EQUILIBRIUM CONSTANT							Enthalpy (KBTU)
	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}	PR
310.65	27.42731	5.53836	1.71461	0.50804	0.17712	0.05986	0.02078	498.53
309.65	27.42705	5.53834	1.71460	0.51349	0.17712	0.05986	0.02078	498.55
308.65	27.42676	5.53831	1.71459	0.51900	0.17712	0.05986	0.02077	498.58
307.65	27.42650	5.53829	1.71458	0.52457	0.17712	0.05986	0.02077	498.60
306.65	27.42626	5.53827	1.71458	0.53019	0.17712	0.05986	0.02077	498.62
305.65	**27.42606**	**5.53826**	**1.71457**	**0.53588**	**0.17711**	**0.05986**	**0.02077**	**498.64**
304.65	27.42583	5.53823	1.71456	0.54162	0.17711	0.05986	0.02077	498.66
303.65	27.42566	5.53822	1.71456	0.54743	0.17711	0.05985	0.02077	498.68
302.65	27.42547	5.53821	1.71455	0.55329	0.17711	0.05985	0.02077	498.70
301.65	27.42533	5.53820	1.71455	0.55922	0.17711	0.05985	0.02077	498.72

Table XV (c). Effect of Change in n-Butane Critical Pressure on Flash Calculation at fixed P and T of a Gas Mixture (SRK).

Critical Pressure (psia)	FLASH CALCULATION EQUILIBRIUM CONSTANT							Enthalpy (KBTU)
	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}	SRK
555.65	27.71762	5.61081	1.73837	0.54317	0.17524	0.05870	0.01991	497.97
554.65	27.71620	5.61067	1.73835	0.54239	0.17524	0.05870	0.01991	497.97
553.65	27.71479	5.61053	1.73832	0.54162	0.17524	0.05870	0.01991	497.96
552.65	27.71338	5.61039	1.73830	0.54086	0.17524	0.05870	0.01991	497.96
551.65	27.71195	5.61025	1.73827	0.54009	0.17524	0.05870	0.01991	497.96
550.65	**27.71049**	**5.61010**	**1.73825**	**0.53933**	**0.17524**	**0.05870**	**0.01991**	**497.96**
549.65	27.70904	5.60996	1.73822	0.53856	0.17524	0.05870	0.01991	497.95
548.65	27.70759	5.60981	1.73820	0.53780	0.17525	0.05870	0.01991	497.95
547.65	27.70611	5.60967	1.73817	0.53705	0.17525	0.05870	0.01991	497.95
546.65	27.70463	5.60952	1.73815	0.53629	0.17525	0.05870	0.01991	497.94

Table XVI (c). Effect of Change in -n-Butane Critical Pressure on Flash Calculation at fixed P and T of a Gas Mixture (PR).

Critical Pressure (psia)	FLASH CALCULATION EQUILIBRIUM CONSTANT							Enthalpy (KBTU)
	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}	PR
555.65	27.43255	5.53886	1.71467	0.53990	0.17711	0.05985	0.02077	498.66
554.65	27.43126	5.53874	1.71465	0.53909	0.17711	0.05985	0.02077	498.65
553.65	27.42999	5.53862	1.71463	0.53829	0.17711	0.05985	0.02077	498.65
552.65	27.42867	5.53850	1.71461	0.53748	0.17711	0.05985	0.02077	498.65
551.65	27.42737	5.53838	1.71459	0.53668	0.17711	0.05986	0.02077	498.64
550.65	**27.42606**	**5.53826**	**1.71457**	**0.53588**	**0.17711**	**0.05986**	**0.02077**	**498.64**
549.65	27.42471	5.53813	1.71455	0.53508	0.17712	0.05986	0.02077	498.64
548.65	27.42339	5.53801	1.71453	0.53429	0.17712	0.05986	0.02077	498.63
547.65	27.42203	5.53788	1.71451	0.53349	0.17712	0.05986	0.02077	498.63
546.65	27.42068	5.53776	1.71449	0.53270	0.17712	0.05986	0.02078	498.63

Table XVII (c). Effect of Change in n-Butane Acentric Factor on Flash Calculation at fixed P and T of a Gas Mixture (SRK).

Acentric Factor (SRK)	FLASH CALCULATION EQUILIBRIUM CONSTANT							Enthalpy (KBTU)
	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}	SRK
0.24710	27.72437	5.61159	1.73856	0.49242	0.17525	0.05870	0.01991	497.75
0.23710	27.72131	5.61126	1.73849	0.50142	0.17525	0.05870	0.01991	497.80
0.22710	27.71843	5.61095	1.73843	0.51061	0.17525	0.05870	0.01991	497.84
0.21710	27.71565	5.61065	1.73837	0.51998	0.17525	0.05870	0.01991	497.88
0.02710	27.71302	5.61037	1.73831	0.52956	0.17525	0.05870	0.01991	497.92
0.19710	**27.71051**	**5.61010**	**1.73825**	**0.53933**	**0.17524**	**0.05870**	**0.01991**	**497.96**
0.18710	27.70813	5.60985	1.73819	0.54930	0.17524	0.05870	0.01991	497.99
0.17710	27.70584	5.60960	1.73814	0.55948	0.17524	0.05870	0.01991	498.03
0.16710	27.70368	5.60936	1.73809	0.56987	0.17524	0.05870	0.01991	498.07
0.15710	27.70163	5.60914	1.73805	0.58048	0.17524	0.05870	0.01991	498.10

Table XVIII (c). Effect of Change in n-Butane Acentric Factor on Flash Calculation at fixed P and T of a Gas Mixture (PR).

Acentric Factor (PR)	FLASH CALCULATION EQUILIBRIUM CONSTANT							Enthalpy (KBTU)
	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}	PR
0.24997	27.43853	5.53940	1.71479	0.48958	0.17712	0.05986	0.02077	498.44
0.23997	27.43580	5.53915	1.71474	0.49844	0.17712	0.05986	0.02077	498.48
0.22997	27.43320	5.53891	1.71469	0.50750	0.17712	0.05986	0.02077	498.52
0.21997	27.43069	5.53868	1.71465	0.51675	0.17712	0.05986	0.02077	498.56
0.20997	27.42832	5.53846	1.71461	0.52621	0.17712	0.05986	0.02077	498.60
0.19997	**27.42606**	**5.53826**	**1.71457**	**0.53588**	**0.17711**	**0.05986**	**0.02977**	**498.64**
0.18997	27.42390	5.53806	1.71453	0.54576	0.17711	0.05986	0.02077	498.68
0.17997	27.42185	5.53787	1.71450	0.55586	0.17711	0.05986	0.02077	498.71
0.16997	27.41989	5.53769	1.71447	0.56619	0.17711	0.05985	0.02077	498.75
0.15997	27.41806	5.53753	1.71443	0.57675	0.17711	0.05985	0.02077	498.79

Table XIX (c). Effect of Change in Heptane Critical Temperature on Flash Calculation at fixed P and T of a Gas Mixture (SRK).

Critical Temperature (°F)	FLASH CALCULATION EQUILIBRIUM CONSTANT							Enthalpy (KBTU)
	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}	SRK
517.87	27.85253	5.62458	1.74089	0.53960	0.17522	0.05867	0.01855	496.10
516.87	27.82412	5.62168	1.74036	0.53954	0.17522	0.05868	0.01881	496.47
515.87	27.79573	5.61878	1.73983	0.53949	0.17523	0.05868	0.01908	496.83
514.87	27.76734	5.61589	1.73930	0.53943	0.17523	0.05869	0.01936	496.20
513.87	27.73892	5.61299	1.73877	0.53938	0.17524	0.05870	0.01963	497.58
512.87	**27.71049**	**5.61010**	**1.73825**	**0.53932**	**0.17524**	**0.05870**	**0.01991**	**497.96**
511.87	27.68208	5.60721	1.73773	0.53927	0.17525	0.05871	0.02019	498.34
510.87	27.65362	5.60432	1.73721	0.53922	0.17526	0.05872	0.02048	498.73
509.87	27.62518	5.60143	1.73669	0.53917	0.17527	0.05873	0.02077	499.12
508.87	27.59670	5.59855	1.73617	0.53913	0.17527	0.05873	0.02107	499.51

Table XX (c). Effect of Change in Heptane Critical Temperature on Flash Calculation at fixed P and T of a Gas Mixture (PR).

Critical Temperature (°F)	FLASH CALCULATION EQUILIBRIUM CONSTANT							Enthalpy (KBTU)
	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}	PR
517.87	27.55644	5.55123	1.71685	0.53608	0.17708	0.05982	0.01938	496.79
516.87	27.53038	5.54864	1.71639	0.53604	0.17708	0.05983	0.01965	497.15
515.87	27.50433	5.54604	1.71594	0.53600	0.17709	0.05983	0.01993	497.52
514.87	27.47824	5.54344	1.71548	0.53596	0.17710	0.05984	0.02021	497.89
513.87	27.45217	5.54085	1.71502	0.53592	0.17711	0.05985	0.02049	498.26
512.87	**27.42606**	**5.53826**	**1.71457**	**0.53588**	**0.17711**	**0.05986**	**0.02077**	**498.64**
511.87	27.39994	5.53566	1.71412	0.53584	0.17712	0.05986	0.02106	499.02
510.87	27.37379	5.53307	1.71367	0.53580	0.17713	0.05987	0.02136	499.41
509.87	27.34766	5.53048	1.71323	0.53577	0.17714	0.05988	0.02166	499.80
508.87	27.32149	5.52789	1.71278	0.53573	0.17715	0.05989	0.02196	500.19

Table XXI (c). Effect of Change in Heptane Critical Pressure on Flash Calculation at fixed P and T of a Gas Mixture (SRK).

Critical Pressure (psia)	FLASH CALCULATION EQUILIBRIUM CONSTANT							Enthalpy (KBTU)
	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}	SRK
401.79	27.99162	5.63977	1.74417	0.54021	0.17534	0.05870	0.02013	498.28
400.79	27.93532	5.63381	1.74297	0.54002	0.17532	0.05870	0.02009	498.21
399,79	27.87907	5.62787	1.74178	0.53984	0.17530	0.05870	0.02004	498.15
398.79	27.82284	5.62193	1.74060	0.53967	0.17528	0.05870	0.02000	498.08
397.79	27.76665	5.61601	1.73942	0.53949	0.17526	0.05870	0.01995	498.02
396.79	**27.71049**	**5.61010**	**1.73825**	**0.53932**	**0.17524**	**0.05870**	**0.01991**	**497.96**
395.79	27.65437	5.60420	1.73709	0.53916	0.17523	0.05870	0.01987	497.89
394.79	27.59829	5.59831	1.73593	0.53900	0.17521	0.05871	0.01982	497.83
393.79	27.54223	5.59243	1.73478	0.53884	0.17420	0.05871	0.01978	497.76
392.79	27.48619	5.58656	1.73364	0.53868	0.17519	0.05872	0.01973	497.70

Table XXII (c). Effect of Change in Heptane Critical Pressure on Flash Calculation at fixed P and T of a Gas Mixture (PR).

Critical Pressure (psia)	FLASH CALCULATION EQUILIBRIUM CONSTANT							Enthalpy (KBTU)
	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}	PR
401.79	27.68170	5.56341	1.71930	0.53649	0.17717	0.05985	0.02100	498.96
400.79	27.63053	5.55836	1.71834	0.53636	0.17715	0.05985	0.02096	498.90
399,79	27.57936	5.55331	1.71739	0.53623	0.17714	0.05985	0.02091	498.83
398.79	27.52824	5.54829	1.71644	0.53611	0.17713	0.05985	0.02087	498.77
397.79	27.47714	5.54326	1.71550	0.53599	0.17712	0.05985	0.02082	498.70
396.79	**27.42606**	**5.53826**	**1.71457**	**0.53588**	**0.17711**	**0.05986**	**0.02077**	**498.64**
395.79	27.37499	5.53325	1.71365	0.53577	0.17711	0.05986	0.02073	498.57
394.79	27.32395	5.52827	1.71273	0.53566	0.17711	0.05986	0.02068	498.51
393.79	27.27297	5.52329	1.71182	0.53556	0.17710	0.05987	0.02064	498.45
392.79	27.22198	5.51833	1.71092	0.53546	0.17710	0.05987	0.02059	498.38

Table XXIII (c). Effect of Change in Heptane Acentric Factor on Flash Calculation at fixed P and T of a Gas Mixture (SRK).

Acentric Factor (SRK)	FLASH CALCULATION EQUILIBRIUM CONSTANT							Enthalpy (KBTU)
	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}	SRK
0.39750	28.59517	5.70245	1.75631	0.54185	0.17545	0.05866	0.01589	492.19
0.38750	28.41623	5.68362	1.75253	0.54127	0.17538	0.05865	0.01663	493.29
0.37750	28.23833	5.66497	1.74883	0.54073	0.17532	0.05865	0.01739	494.41
0.36750	28.06141	5.64650	1.74522	0.54022	0.17528	0.05866	0.01820	495.56
0.35750	27.88544	5.62821	1.74169	0.53975	0.17525	0.05868	0.01903	496.74
0.34750	**27.71049**	**5.61010**	**1.73825**	**0.53933**	**0.17524**	**0.05870**	**0.01991**	**497.96**
0.33750	27.53654	5.59217	1.73489	0.53893	0.17525	0.05873	0.02083	499.20
0.32750	27.36357	5.57443	1.73163	0.53858	0.17528	0.05877	0.02178	500.48
0.31750	27.19164	5.55686	1.72845	0.53827	0.17532	0.05882	0.02278	501.79
0.30750	27.01859	5.53920	1.72528	0.53797	0.17537	0.05887	0.02383	502.99

Table XXIV (c). Effect of Change in Heptane Acentric Factor on Flash Calculation at fixed P and T of a Gas Mixture (PR).

Acentric Factor (PR)	FLASH CALCULATION EQUILIBRIUM CONSTANT							Enthalpy (KBTU)
	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}	PR
0.39907	28.22601	5.61816	1.72950	0.53774	0.17721	0.05979	0.01669	492.96
0.38907	28.06504	5.60193	1.72637	0.53730	0.17716	0.05979	0.01744	494.03
0.37907	27.90456	5.58583	1.72331	0.53689	0.17712	0.05979	0.01822	495.14
0.36907	27.74454	5.56985	1.72033	0.53652	0.17710	0.05981	0.01903	496.27
0.35907	27.58504	5.55399	1.71742	0.53618	0.17710	0.05983	0.01988	497.44
0.34907	**27.42605**	**5.53826**	**1.71457**	**0.53588**	**0.17711**	**0.05986**	**0.02077**	**498.64**
0.33970	27.26757	5.52265	1.71180	0.53561	0.17714	0.05989	0.02170	499.87
0.32907	27.10964	5.50717	1.70911	0.53538	0.17719	0.05993	0.02268	501.14
0.31907	26.95204	5.49179	1.70648	0.53518	0.17725	0.05998	0.02369	502.43
0.30907	26.77620	5.47394	1.70321	0.53482	0.17726	0.06001	0.02475	502.44

d) Binary Interaction Parameter

The bubble point temperature and the dew point temperature calculations at 100 psia (698.48 kPa) for pure methane, ethane, propane n-butane n-pentane were performed using the SRK and the PR equations of state. Arbitrary changes in the binary interaction parameter were made for each of the pure hydrocarbons. Calculations were carried out to see how the change in the interaction parameter influenced calculation results. Tables I (d) through V (d) show results for the bubble and dew point calculations.

The effect of increasing the binary interaction parameter on the calculated bubble and dew point for methane is shown in Table I (d). Increasing the binary interaction parameter (from **0.0** – 0.10) did not change the calculated bubble point nor the calculated dew point for methane.

The effect of increasing the binary interaction parameter on the calculated bubble and dew point for ethane is shown in Table II (d). Increasing the binary interaction parameter from (**0.0** – 0.10) did not change the calculated bubble point nor the calculated dew point for ethane.

The effect of increasing the binary interaction parameters on the calculated bubble and dew point for propane is shown in Table III (d). Increasing the binary interaction parameter from (**0.0** – 0.10) did not change the calculated bubble point nor the calculated dew point for propane.

Table I (d). Effect of Change in Interaction Parameter on Calculated Bubble and Dew Point of Methane.

Interaction Parameter (kij)	Bubble Point Temperature (°F)	Enthalpy (kBTU)	Dew Point Temperature (°F)	Enthalpy (kBTU)
0.00	**-205.83**	**-128.51**	**-205.83**	**179.40**
0.01	-205.83	-128.51	-205.83	179.40
0.02	-205.83	-128.51	-205.83	179.40
0.03	-205.83	-128.51	-205.83	179.40
0.04	-205.83	-128.51	-205.83	179.40
0.05	-205.83	-128.51	-205.83	179.40
0.06	-205.83	-128.51	-205.83	179.40
0.07	-205.83	-128.51	-205.83	179.40
0.08	-205.83	-128.51	-205.83	179.40
0.09	-205.83	-128.51	-205.83	179.40
0.10	-205.83	-128.51	-205.83	179.40

Table II (d). Effect of Change in Interaction Parameter on Calculated Bubble and Dew Point of Ethane.

Interaction Parameter (kij)	Bubble Point Temperature (°F)	Enthalpy (kBTU)	Dew Point Temperature (°F)	Enthalpy (kBTU)
0.00	**-47.23**	**-209.14**	**-47.23**	**338.55**
0.01	-47.23	-209.15	-47.23	338.55
0.02	-47.23	-209.15	-47.23	338.55
0.03	-47.23	-209.14	-47.23	338.55
0.04	-47.23	-209.14	-47.23	338.55
0.05	-47.23	-209.14	-47.23	338.55
0.06	-47.23	-209.14	-47.23	338.55
0.07	-47.23	-209.14	-47.23	338.55
0.08	-47.23	-209.14	-47.23	338.55
0.09	-47.23	-209.14	-47.23	338.55
0.10	-47.23	-209.14	-47.23	338.55

Table III (d). Effect of Change in Interaction Parameter on Calculated Bubble and Dew Point of Propane.

Interaction Parameter (kij)	Bubble Point Temperature (°F)	Enthalpy (kBTU)	Dew Point Temperature (°F)	Enthalpy (kBTU)
0.00	**54.32**	**-132.65**	**54.32**	**552.57**
0.01	54.32	-132.65	54.32	552.57
0.02	54.32	-132.65	54.32	552.57
0.03	54.32	-132.65	54.32	552.57
0.04	54.32	-132.65	54.32	552.57
0.05	54.32	-132.65	54.32	552.57
0.06	54.32	-132.65	54.32	552.57
0.07	54.32	-132.65	54.32	552.57
0.08	54.32	-132.65	54.32	552.57
0.09	54.32	-132.65	54.32	552.57
0.10	54.32	-132.65	54.32	552.57

The effect of increasing the binary interaction parameter on the calculated bubble and dew point for n-butane is shown in Table IV (d). Increasing the binary interaction parameter from (**0.0** – 0.10) did not change the calculated bubble point nor the calculated dew point for n-butane.

Table IV (d). Effect of Change in Interaction Parameter on Calculated Bubble and Dew Point of n-Butane.

Interaction Parameter (kij)	Bubble Point Temperature (°F)	Enthalpy (kBTU)	Dew Point Temperature (°F)	Enthalpy (kBTU)
0.00	**144.61**	**145.07**	**144.61**	**951.81**
0.01	144.61	145.07	144.61	951.81
0.02	144.61	145.07	144.61	951.81
0.03	144.61	145.07	144.61	951.81
0.04	144.61	145.07	144.61	951.81
0.05	144.61	145.07	144.61	951.81
0.06	144.61	145.07	144.61	951.81
0.07	144.61	145.07	144.61	951.81
0.08	144.61	145.07	144.61	951.81
0.09	144.61	145.07	144.61	951.81
0.10	144.61	145.07	144.61	951.81

The effect of increasing the binary interaction parameter on the calculated bubble and dew point for n-pentane is shown in Table V (d). Increasing the binary interaction parameter from (**0.0** – 0.10) did not change the calculated bubble point nor the calculated dew point for n-pentane.

Table V (d). Effect of Change in Interaction Parameter on Calculated Bubble and Dew Point of n-Pentane.

Interaction Parameter (kij)	Bubble Point Temperature (°F)	Enthalpy (kBTU)	Dew Point Temperature (°F)	Enthalpy (kBTU)
0.00	**223.08**	**505.43**	**223.08**	**1416.02**
0.01	223.08	505.43	223.08	1416.02
0.02	223.08	505.43	223.08	1416.02
0.03	223.08	505.43	223.08	1416.02
0.04	223.08	505.43	223.08	1416.02
0.05	223.08	505.43	223.08	1416.02
0.06	223.08	505.43	223.08	1416.02
0.07	223.08	505.43	223.08	1416.02
0.08	223.08	505.43	223.08	1416.02
0.09	223.08	505.43	223.08	1416.02
0.10	223.08	505.43	223.08	1416.02

Binary Mixture

The bubble point, dew point and flash calculations were performed for equimolar binary mixtures of methane and ethane, methane and propane and n-butane and n-pentane. The binary mixture bubble point and the dew point temperature calculations were performed at 100 psia (698.48 kPa). Changes in the interaction parameters were made for each mixture. Tables VI (d) through VIII (d) show the results for bubble and dew point calculations. The flash calculations were performed at fixed L/F = 0.5 and at fixed pressure of 100 psia. The results are presented in Tables IX (d).

The effect of changing the interaction parameter on the calculated bubble and dew point for a methane and ethane binary mixture is shown in Table VI (d). Increasing the interaction parameter, decreases the calculated bubble and dew point for the mixture.

The effect of changing the interaction parameter on the calculated bubble and dew point for a methane and propane binary mixture is shown in Table VII (d). Increasing the interaction parameter decreases the calculated bubble and dew point for the mixture.

The effect of changing the interaction parameter on the calculated bubble and dew point for a n-butane and n-pentane binary mixture is shown in Table VIII (d). Increasing the interaction parameter decreases the calculated bubble and dew point for the mixture.

Table VI (d). Effect of Change in Interaction Parameter on Calculated Bubble and Dew Point of Equimolar Mixture of Methane and Ethane.

Interaction Parameter (kij)	Bubble Point Temperature (°F)	Equilibrium Constant		Enthalpy (kBTU)	Dew Point Temperature (°F)	Equilibrium Constant		Enthalpy (kBTU
		CH_4	C_2H_6			CH_4	C_2H_6	
0.00	**-180.56**	1.96992	0.03008	**-274.65**	**-81.51**	8.31369	0.53200	**294.73**
0.01	-182.07	1.97121	0.02879	-274.41	-81.64	8.73395	0.53036	294.70
0.02	-183.60	1.97247	0.02753	-274.19	-81.76	9.18060	0.52880	294.67
0.03	-185.13	1.97370	0.02630	-273.97	-81.88	9.65518	0.52731	294.66
0.04	-186.67	1.97489	0.02511	-273.75	-81.99	10.15932	0.52588	294.65
0.05	-188.22	1.97606	0.02394	-273.55	-82.09	10.69474	0.52452	294.64
0.06	-189.78	1.97719	0.02281	-273.35	-82.18	11.26325	0.52323	294.65
0.07	-191.35	1.97829	0.02171	-273.16	-82.27	11.86677	0.52199	294.65
0.08	-192.93	1.97936	0.02064	-272.97	-82.36	12.50729	0.52082	294.67
0.09	-194.52	1.98040	0.01960	-272.79	-82.43	13.18698	0.51970	294.69
0.10	-196.12	1.98141	0.01859	-272.62	-82.51	13.90799	0.51865	294.72

Table VII (d). Effect of Change in Interaction Parameter on Calculated Bubble and Dew Point of Equimolar Mixture of Methane and Propane.

Interaction Parameter (kij)	Bubble Point Temperature (°F)	Equilibrium Constant		Enthalpy (kBTU)	Dew Point Temperature (°F)	Equilibrium Constant		Enthalpy (kBTU)
		CH_4	C_3H_8			CH_4	C_3H_8	
0.00	**-183.45**	1.99897	0.00103	**-404.13**	**10.65**	16.69924	0.51543	**424.91**
0.01	-185.45	1.99907	0.00093	-404.72	10.61	17.33018	0.51485	424.95
0.02	-187.48	1.99916	0.00084	-405.31	10.57	17.98703	0.51430	425.00
0.03	-189.51	1.99924	0.00076	-405.91	10.53	18.67078	0.51376	425.04
0.04	-191.56	1.99932	0.00068	-406.52	10.49	19.38252	0.51324	425.09
0.05	-193.61	1.99939	0.00061	-407.14	10.46	20.12331	0.51274	425.15
0.06	-195.69	1.99946	0.00054	-407.77	10.43	20.89428	0.51226	425.20
0.07	-197.78	1.99952	0.00048	-408.40	10.40	21.69667	0.51179	425.26
0.08	-199.88	1.99957	0.00043	-409.05	10.37	22.53172	0.51135	425.33
0.09	-201.99	1.99962	0.00038	-409.70	10.34	23.40066	0.51092	425.39
0.10	-204.12	1.99967	0.00034	-410.37	10.32	24.30486	0.51050	425.46

Table VIII (d). Effect of Change in Interaction Parameter on Calculated Bubble and Dew Point of Equimolar Mixture of n-Butane and n-Pentane.

Interaction Parameter (kij)	Bubble Point Temperature (°F)	Equilibrium Constant		Enthalpy (kBTU)	Dew Point Temperature (°F)	Equilibrium Constant		Enthalpy (kBTU)
		C_4H_{10}	C_5H_{12}			C_4H_{10}	C_5H_{12}	
0.00	**176.79**	1.39712	0.60288	**276.38**	**192.47**	1.61658	0.72390	**1196.51**
0.01	174.98	1.40061	0.59939	274.64	191.15	1.65346	0.71674	1192.59
0.02	173.17	1.40415	0.59585	272.88	189.85	1.69404	0.70937	1188.74
0.03	171.35	1.40772	0.59228	271.12	188.57	1.73883	0.70180	1184.96
0.04	169.52	1.41133	0.58867	269.35	187.31	1.78837	0.69404	1181.27
0.05	167.68	1.41498	0.58502	267.57	186.08	1.84330	0.68611	1177.66
0.06	165.84	1.41867	0.58133	265.77	184.87	1.90438	0.67801	1174.15
0.07	163.98	1.42242	0.57758	263.97	183.69	1.97240	0.66979	1170.73
0.08	162.12	1.42618	0.57382	262.16	182.55	2.04831	0.66147	1167.43
0.09	160.25	1.42998	0.57002	260.34	181.44	2.13315	0.65308	1164.24
0.10	158.37	1.43385	0.56615	258.52	180.36	2.22810	0.64467	1161.18

The effect of changing the interaction parameter on the calculated flash temperature for the binary mixture of n-butane and n-pentane is shown in Table IV (o). Increasing the interaction parameter decreases the calculated flash temperature for the mixture.

Table IX (d). Effect of Changes in Interaction Parameter on Flash Calculations at fixed P and L/F=0.5 of Equimolar Mixture of n-Butane and n-Pentane.

Interaction parameter	Liquid Mole Fraction		Flash Temperature (°F)	Equilibrium Constant		Enthalpy (kBTU)
	n-Butane	n-Pentane		n-Butane	n- Pentane	
0.00	**0.3988**	**0.6012**	**184.84**	**1.50783**	**0.66321**	**731.77**
0.01	0.3961	0.6039	183.09	1.52469	0.65587	727.89
0.02	0.3933	0.6067	181.33	1.54255	0.64827	723.96
0.03	0.3904	0.6096	179.56	1.56152	0.64040	719.95
0.04	0.3873	0.6127	177.77	1.58169	0.63223	715.86
0.05	0.3841	0.6159	175.97	1.60320	0.62375	711.69
0.06	0.3808	0.6192	174.15	1.62616	0.61495	707.43
0.07	0.3773	0.6227	172.31	1.65069	0.60579	703.06
0.08	0.3735	0.6265	170.44	1.67703	0.59629	698.58
0.09	0.3696	0.6304	168.56	1.70533	0.58639	693.97
0.10	0.3655	0.6345	166.64	1.73581	0.57609	689.23

CHAPTER V

DISCUSSION

Pure Hydrocarbons

Changes in critical temperature, critical pressure and acentric factor on the calculated bubble and dew point temperature for pure hydrocarbons show the following:

The effect of changing the critical temperature on the calculated bubble and dew point for methane are shown in Tables I (a) and IV (a). Increasing the critical temperature by 1 °F, increases the calculated bubble and dew point for methane by about 0.75°F for both the SRK and the PR. Increasing the critical temperature by 5°F, increases the bubble and dew point by 3.7 °F for both the SRK and the PR. Lowering the critical temperature lowers the calculated bubble and dew point by almost the same amount, so within the limited temperature range, changes are linear. The changes are identical in magnitude for both the SRK and the PR equations of state.

The effect of changing the critical temperature on the calculated bubble and dew point for ethane are shown in Tables VII (a) and X (a). Increasing the critical temperature by 1 °F, increases the calculated bubble and dew point for ethane by about 0.75°F for both the SRK and. Increasing the critical temperature by 5 °F, increases the bubble and dew point temperature by about 3.75 °F for both the SRK and. Lowering the critical temperature lowers the calculated bubble and dew point by almost the same amount, so within the limited temperature range, changes are linear.

The effect of changing the critical temperature on the calculated bubble and dew point for propane are shown in Tables XIII (a) and XVI (a). Increasing the critical temperature by 1 °F, increases the calculated bubble and dew point for propane by 0.77°F for both the SRK and the PR. Increasing the critical temperature by 5°F, increases the bubble and dew point temperature by 3.86 °F for both the SRK and the PR. Lowering the critical temperature lowers the calculated bubble and dew point by almost the same amount, so within the limited temperature range, changes are linear.

The effect of changing methane critical pressure on the calculated bubble and dew point are shown in Tables II (a) and V (a). An increase in critical pressure of 5 psia, decreases the calculated bubble and dew point temperature by only 0.26 °F for both the SRK and the PR. Lowering the critical pressure increases the calculated bubble and dew point temperature by almost the amount, so within the limited temperature range, changes are linear. An increase in critical pressure of one psi, decreases the bubble and dew point calculations by 0.05 °F for both the SRK and the PR.

The effect of changing ethane critical pressure on the calculated bubble and dew point are shown in Tables VIII(a) and XI (a). An increase in critical pressure of 5 psi, decreases the calculated bubble and dew point temperature by only 0.37 °F for both the SRK and the PR. Lowering the critical pressure increases the calculated bubble point by almost the same amount, so within the limited temperature range, changes are linear. An increase in critical pressure of one psia , decreases the bubble and dew point calculations by about 0.07 °F for both the SRK and PR. Results for both equations are again similar, but the change is much smaller.

The effect of changing propane critical pressure on the calculated bubble and dew point are shown in Tables XIII (a) and XVII (a). An increase in critical pressure of 5 psi, decreases the calculated bubble and dew point temperature by only 0.52 °F for both the SRK and the PR. Lowering the critical pressure increases the calculated bubble point by almost the same amount, so within the limited temperature range, changes are linear. An increase in the critical pressure of one psi , decreases the bubble and dew point calculations by about 0.10 °F for both the SRK and PR. Results for both equations are again similar, but the change is much smaller.

The impact of changing the acentric factor on the calculated bubble and dew point for methane are shown in Tables III (a) and VI (a). Changing the acentric factor for the SRK from (**0.0039** to 0.0049), increases the bubble and dew point temperature by 0.07 °F. Changing the acentric factor for the PR from (**0.014** to 0.024) increases the bubble and dew point temperature by 0.67 °F.

The impact of changing the acentric factor on the calculated bubble and dew point for ethane are shown in Tables IX (a) and XII (a). Changing the acentric factor for the SRK from (**0.0944** to 0.1044) increases the bubble and dew point temperature by about 0.90 °F. Changing the acentric factor for the PR from (**0.09947** to 0.10947) increases the bubble and dew point temperature by about 0.90 °F. The changes are identical in magnitude for both the SRK and the PR equations of state. Results for both equations are again similar.

The impact of changing the acentric factor on the calculated bubble and dew point for propane are shown in Tables XV (a) and XVIII (f). Changing the acentric factor for the SRK from (**0.1497** to 0.1597) increases the bubble and dew point temperature by about 0.96 °F. Changing the acentric factor for the PR from (**0.15355** to 0.16355) increases the bubble point temperature by about 0.96 °F. The changes are identical in magnitude for both the SRK and the PR equations of state. Results for both equations are again similar.

These comparisons show that SRK and PR predictions are clearly altered when changes are made in the physical properties, although, the changes made in critical temperature, critical pressure and the acentric factor are small for both equations. Changes in critical temperature have a more significant effect on the predictions of bubble and dew point temperatures than the change in the critical pressure or the acentric factor.

Binary Mixture

The impact of changes in critical temperature, critical pressure and acentric factor for an equimolar binary mixture of n-butane and n-pentane are presented in Tables I (b), through XII (b). The flash calculations were performed at fixed L/F of 0.5 and a pressure of 100 psi and results are shown in Tables XIII (b) through XX (b).

The effect of changing the critical temperature of n-butane on the calculated bubble point for the binary mixture are shown in Tables I (b). Increasing the critical temperature of n-butane by 1 °F, increases the calculated bubble point for the mixture by about 0.55°F for both the SRK and the PR.

Increasing the critical temperature of n-butane by 5°F, increases the bubble point temperature for the mixture by about 2.70 °F for both the SRK and the PR. Lowering the critical temperature lowers the calculated bubble point by almost the same amount, so within the limited temperature range, changes are linear.

The effect of changing the critical temperature of n-pentane on the calculated bubble point for the binary mixture are shown in Tables II (b). Increasing the critical temperature of n-pentane by 1 °F, increases the calculated bubble point for the mixture by about 0.25°F for both the SRK and the PR. Increasing the critical temperature of n-butane by 5°F, increases the bubble point temperature for the mixture by about 1.25 °F for both the SRK and the PR. Lowering the critical temperature lowers the calculated bubble point by almost the same amounts, so within the limited temperature range, changes are linear.

The effect of changing the critical temperature of n-butane on the calculated dew point for the binary mixture are shown in Tables VII (b). Increasing the critical temperature of n-butane by 1 °F, increases the calculated dew point for the mixture by about 0.23°F for both the SRK and the PR. Increasing the critical temperature of n-butane by 5°F, increases the dew point temperature for the mixture by 1.16 °F for both the SRK and the PR. Lowering the critical temperature lowers the calculated dew point by almost the same amounts.

The effect of changing the critical temperature of n-pentane on the calculated dew point for the binary mixture are shown in Tables VIII (b). Increasing the critical temperature of n-butane by 1 °F, increases the calculated dew point for the mixture by about 0.56°F for both the SRK and the PR.

Increasing the critical temperature of n-butane by 5°F, increases the dew point temperature for the mixture by 2.83 °F for both the SRK and the PR. Lowering the critical temperature lowers the calculated dew point by almost the same amounts, so within the limited temperature range, changes are linear.

The effect of changing the critical pressure of n-butane on the calculated bubble point for the binary mixture are shown in Tables III (b). Increasing n-butane critical pressure of 5 psi, decreases the calculated bubble point temperature for the mixture by 0.48°F for both the SRK and the PR. Lowering n-butane critical pressure of 5 psi, increases the bubble point temperature for the mixture by almost the same amount. An increase in the critical pressure of one psi decreases the bubble point calculation by about 0.10 °F for both the SRK and the PR.

The effect of changing n-pentane critical pressure on the calculated bubble point of the mixture are shown in Table IV (b). Increasing n-pentane critical pressure of 5 psi, decreases the bubble point temperature of the mixture by about 0.28 °F for both the SRK and the PR. An increase in the critical pressure of one psi decreases the bubble point of the mixture by 0.05 °F for both the SRK and the PR. Lowering the critical pressure increases the calculated bubble point by almost the same amount, so within the limited temperature range, changes are linear.

The effect of changing the critical pressure of n-butane on the calculated dew point for the binary mixture are shown in Tables IX (b). Increasing n-butane critical pressure of 5 psi, decreases the calculated dew point temperature for the mixture by about 0.20 °F for both the SRK and the PR. An increase in the critical pressure of one psi decreases the dew point calculation by 0.04 °F for both the SRK and the PR.

The effect of changing n-pentane critical pressure on the calculated dew point of the mixture are shown in Table X (b). Increasing n-pentane critical pressure of 5 psi, decreases the dew point temperature of the mixture by about 0.56 °F for both the SRK and the PR. An increase in the critical pressure of one psi decreases the dew point of the mixture by about 0.10 °F for both the SRK and the PR. Lowering the critical pressure increases the calculated dew point by almost the same amount, so within the limited temperature range, changes are linear.

The effect of changing the acentric factor of n-butane and n-pentane on the calculated bubble point for the binary mixture are shown in Tables XI (b) and XII (b).

Increasing the acentric factor for n-butane from (**0.19710** to 0.20710) increases the bubble point temperature of the mixture by about 0.55°F for the SRK. Changing the acentric factor for the PR from (**0.19997** to 0.20997) increases the bubble point for the mixture by the same amount, so within the limited temperature range, changes are linear. Changing the acentric factor n-pentane from (**0.2490** to 0.2590) increases the bubble point by 0.40 °F for the SRK. Increasing the acentric factor for the PR from (**0.24914** to 0.25914) increases the bubble point of the mixture by the same amount, so within the limited temperature range, changes are linear.

The effect of changing the acentric factor of n-butane and n-pentane on the calculated dew point for the binary mixture are shown in Tables XI (b) and XII (b). Increasing the acentric factor for n-butane from (**0.19710** to 0.20710) increases the dew point temperature of the mixture by about 0.20°F for the SRK.

Increasing the acentric factor for the PR from (**0.19997** to 0.20997) increases the dew point for the mixture by the same amount. Increasing the acentric factor for n-pentane from (**0.2490** to 0.2590) increases the dew point by about 0.82 °F for the SRK. Changing the acentric factor for the PR from (**0.24914** to 0.25914) increases the dew point of the mixture by the same amount The effect of changing the acentric factor of n-pentane on the calculated dew point temperature of the mixture.

The effect of changing the critical temperature of n-butane on the calculated flash temperature for the binary mixture are shown in Table XIII (b). Increasing the critical temperature of n-butane by 1 °F, increases the calculated flash temperature by 0.38 °F for both the SRK and the PR.

Increasing the critical temperature by 5 °F, increases the flash temperature by about 1.90 °F for both the SRK and the PR. Lowering the critical temperature lowers the calculated flash temperature by almost the same amount, so within the limited temperature range, changes are linear.

The effect of changing the critical temperature of n-pentane on the calculated flash temperature for the binary mixture are shown in Table XIV (b). Increasing the critical temperature of n-pentane by 1 °F, increases the calculated flash temperature by 0.40 °F for both the SRK and the PR. Increasing the critical temperature of n-pentane by 5 °F, increases the calculated flash temperature by about 2.10 °F for both the SRK and the PR. Lowering the critical temperature lowers the calculated flash temperature by almost the same amounts, so within the limited temperature range, changes are linear.

The impact of changing the critical pressure of n-butane on the calculated flash temperature for the binary mixture are shown in Table XV (b). Increasing n-butane critical pressure of 5 psi, decreases the calculated flash temperature for the mixture by about 0.30°F for both the SRK and °F the PR. Lowering the critical pressure of 5 psi, increases the flash temperature for the mixture by almost the same amount. An increase in the critical pressure of one psi decreases the flash temperature calculation by 0.07 °F for both the SRK and the PR.

The effect of changing n-pentane critical pressure on the calculated flash temperature of the mixture are shown in Table XVI (b). Increasing n-pentane critical pressure of 5 psi, decreases the flash temperature by 0.43 °F for both the SRK and the PR.

An increase in the critical pressure of one psi decreases the flash temperature of the mixture by 0.09 °F for both the SRK and the PR. Lowering the critical pressure increases the calculated flash temperature by almost the same amount.

The effect of changing the acentric factor of n-butane and n-pentane on the calculated flash temperature for the binary mixture are shown in Tables XVII (b), XVIII (b), XIX (b) and XX (b). Changing the acentric factor for n-butane from (**0.19710** to 0.20710) increases the calculated flash temperature of the mixture by 0.35°F for the SRK. Changing the acentric factor for the PR from (**0.19997** to 0.20997) increases the flash temperature by 0.05 °F. Changing n-pentane acentric factor from (**0.2490** to 0.2590) increases the flash temperature by about 0.60 °F for the SRK. Increasing the acentric factor for the PR from (**0.24914** to 0.25914) increases the flash of the mixture by about 0.60 °F.

Similar behaviors are shown for the calculated bubble point, dew point and flash temperature for the binary mixture of n-butane and n-pentane. Increasing the critical temperature of either compound, increases the mixture calculated bubble point, dew point and flash temperature. Increasing the critical pressure, decreases the mixture calculated bubble point, dew point and flash temperature. An increase in the acentric factor increases the mixture calculated bubble point, dew point and flash temperature.

The results for flash calculations show that the predicted equilibrium constants also changed because of the change in calculated bubble point, dew point and flash temperature. These comparisons show that SRK and PR predictions are clearly altered when changes are made in the physical properties, although, the changes made in critical temperature, critical pressure and the acentric factor are small for both equations.

Changes in critical temperature have a more significant effect on the predictions of bubble and dew point temperatures than the change in the critical pressure or the acentric factor.

Multicomponent Mixture

Flash calculations were performed for the multicomponent gas mixture at 100 psia and 100 °F. Changes in critical temperature, critical pressure and acentric factor were made separately for methane, ethane, n-butane, n-pentane and heptane. Table I (c) through VI (c) show the results of changing the critical temperature, critical pressure and acentric factor of methane on the multicomponent flash. More detailed output for one multicomponent flash calculation is shown in Appendix A.

Tables VII (c) through XXIV (c) show the effect of changing the critical temperature, critical pressure and acentric factor for the other components in the multicomponent mixture. Changing a property for one component in the mixture causes for that component a change in K-value in the same way as for a pure component. This forces a change in the K-value for all components in the mixture and changes the results of the equilibrium calculation. The calculations summarized in Tables I (c) through XXIV (c) clearly show that even small changes in pure component properties will cause changed calculation results for both the SRK and the PR equation of state.

In this work, changes in critical temperature have a more significant effect on the predictions of equilibrium conditions than an equal magnitude change in critical pressure or acentric factor, but none of the changes may *a priori* be considered negligible.

Binary Interaction Parameter

Bubble point temperature and dew point temperature calculations at 100 psia (698.48 kPa) for pure methane, ethane, propane, n-butane, and n-pentane were performed using the SRK and the PR equations of state. Arbitrary changes in the binary interaction parameter were made for each of the pure hydrocarbons to see how the changes in the interaction parameters influenced the calculated temperature. Tables I (d) through V (d) summarize the calculation results.

Changing the binary interaction parameter (k_{ij}) has no discernible effect on either the calculated bubble point or dew point for single pure component hydrocarbons. This is an expected result because the term "interaction parameter" implies that at least two components are present.

Bubble point, dew point and flash calculations were carried out for equimolar binary mixtures of methane and ethane, methane and propane and n-butane and n-pentane at 100 psia (698.48 kPa). Changes in the interaction parameter were made for each mixture. The SRK and the PR equations used assume interaction parameters are zero (0.0) for all paraffin aliphatic hydrocarbons. Bubble point and dew point calculation results are summarized in Tables VI (d) through VIII (d) and the flash calculations (performed at fixed L/F = 0.5 and 100 psia pressure) are summarized in Table IX (d).

The result of changing the interaction parameter on the calculated bubble and dew point for methane and ethane binary mixture is shown in Table VI (d), in Table VII (d) for methane-propane binary and in Table VIII (d) for the n-butane-n-pentane binary.

Increasing the interaction parameter, decreases the calculated bubble point and the dew point for each mixture.

The effect of changing the interaction parameter on the calculated flash temperature for the binary mixture of n-butane and n-pentane is shown in Table IX (d). Increasing the interaction parameter, decreases the calculated flash temperature for the mixture.

These comparisons show that the binary interaction parameter has no impact on the calculated bubble point and dew point temperature for pure components. However, the binary interaction parameter has a significant impact on the calculated results for both binary and multicomponent mixtures. Cubic equations of state calculate the properties of a fluid mixture as if it consisted of one imaginary component with properties "averaged" by the mixing rule over all components in the mixture. If the fluid is a mixture, the parameters a and b of the imaginary component are calculated from the pure component parameters using the mixing rule.

The critical properties of pure compounds are important as input parameters for cubic equation of state. The SRK and the PR predictions are clearly altered when changes are made in the physical properties. Changes in the critical temperature have more significant effect on the predictions than changes in critical pressure or acentric factor. The values for the physical properties originally used when the equation of state programs were written should not be altered even if more recently measured values appear to be improved or more precise.

Enthalpy calculation

For enthalpies the SRK and the PR equations use the enthalpy departure function to obtain enthalpies from ideal gas values. Suggestions have been made (Hamam, 1995) that, when developing constants for a mixture separate values of the interaction parameter (k_{ij}) for vapor-liquid equilibrium and for enthalpy. In each calculation reported in this thesis the calculated enthalpy is also reported. For single components, all enthalpy variations in any of the reported calculations can be accounted for by temperature variation. There are no composition effects. For mixtures the k_{ij} causes a significant change in the temperature, but there also appears to be an additional effect cause by the entry of the non-zero k_{ij} directly into the mixing rule calculation of mixture enthalpy.

Adachi and Sugie (1) in their study of the effect of cubic equation of state parameters on enthalpy departure calculations, concluded that the covolume parameter, *b*, in both the SRK and the PR is the controlling factor in enthalpy calculations. According to their study and from the *b* parameter equations [12], [18] and [25], there is no binary interaction parameter involved in the calculation of this parameter for either pure component or the mixture. However, the parameter *a* for mixtures in equation [26] has the value of the interaction parameter and, therefore, the enthalpies for mixtures change when interaction parameter is not zero.

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

The following conclusions are based on analysis of output from several hundred calculations of both single component and mixture calculations of vapor-liquid equilibrium and accompanying phase enthalpies.

Conclusions

The critical properties of pure compounds are important as input parameters for cubic equations of state. The SRK and the PR equations of state calculation results are altered when changes are made in the physical properties. For pure light hydrocarbon components increasing the critical temperature or the acentric factor increases the calculated bubble point or dew point temperature; increasing the critical pressure decreases the calculated bubble point or dew point temperature. Conversely, lowering the critical temperature lowers the calculated bubble point or dew point temperature. Within the limited temperature range covered in this work the changes are linear. Similar behaviors are shown for the calculated bubble and dew point for binary mixtures of light hydrocarbons.

Relatively changes in the critical temperature have a more significant effect on the calculations than do changes in critical pressure or acentric factor. Changes in the critical pressure have negligible effect on the calculated bubble point or dew point.

The results for mixtures show that the phase behavior calculations of the SRK and the PR equations of state depend on the pure fluid properties. The predicted equilibrium constants are also dependent on these changes.

The binary interaction parameter has no effect on the predictions for pure components. However, the binary interaction parameter does have an effect on the calculated results for mixtures. When an interaction parameter is to be used to provide better agreement between calculated and experimentally measured VLE data for any mixture, available enthalpy data must be included in the regression calculations to determine the optimum value for k_{ij} .

Recommendations

The values for the physical properties originally used when the equation of state programs were written should not be altered, even if newly available values appear to be improved or more precise in measurement. Changing pure component property values requires that all pure component and mixture date for the changed components must then be recalculated and reevaluated.

The binary interaction parameter has a significant effect on the predicted properties of mixtures. Use of an interaction parameter is recommended only where calculations without an interaction parameter are clearly deficient and lacking in accuracy.

Because of the impact the binary interaction parameter has on mixture enthalpy calculations any effort to develpo an optimum k_{ij} fot a mixture should incorporate a weighting procedure such as that recommended by Moshfeghian and Maddox (10).

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APPENDIX A

Interpreting Equation of State Calculation Results

One of the difficulties in using either the SRK or the PR equation is the difficulty of being certain the computer program has reached a "good" solution. When the user is working with a mixture of two or more components and both vapor and liquid phases are present in the computed solution the solution reached should always be correct. Most programs are forced to a solution even if there is only one phase present. For a single component there may be confusion as to whether the solution is correct. Look at the results in Table A1 where the results are shown for a "good" solution for the bubble point temperature at 100 psia for n-butane. The K-value of butane is 1.0 as would be expected.

Now look at Table A2, which shows the same calculation except the calculated bubble point temperature is 500°F. The K value for n-butane is 1.0, but obviously the solution cannot be correct.

Tables A3 and A4 display one technique for avoiding this problem and allowing the user to be sure a proper solution has been reached. Iso pentane has been introduced to produce a binary mixture, but with zero (0.0) concentration of i-pentane. Table A3 shows the "good" bubble point calculation. The K-value for n-butane is 1.0, but the K-value for i-pentane is 0.489. The solution in Table A4 is not "good" because the K-value for n-butane and for I-pentane is each 1.0, a physical impossibility.

Tables A5 and A6 show the same kind of results for a binary mixture of normal butane and normal pentane. The difference is that the "bad" solution is indicated by K-values that are arbitrarily close to 1.0 rather than being identically equal to 1.0.

Typical calculation results

Tables A1 through A6 are typical of the calculation results used in this work. The information desired for this work is provided, but so is a large quantity of data that is not directly required, once the validity of the particular solution was assured. For this reason the necessary and important information for this work was extracted and presented in summary form as shonw in Tables I(a) through IX(d) in Chapter IV. The several hundred pages of direct computer are still in hand, and will be kept together for several years in case questions arise.

Calculated Results

Though not of specific interest to the main subject of this work, the response of the equation of state calculations to changes made in pure component properties was intriguing. Consider the changes made in critical temperature for a pure component. Bubble point calculations using the "new" value of critical temperature altered the shape of the bubble point curve as shown in Figure A1. The equation of state to seek to calculate a bubble (dew) point curve that matches the "new" value for the component critical temperature. Study of the equations for the SRK (Chapter II) reveals no readily apparent reason, but the change in the pure component property reacts on the equations to produce this result.

Table A1.

```
 This EZ*THERMO is licensed to:
    Dr. R. N. Maddox
    CEC, Inc.
    June 23, 1997

BUBBLEPOINT OF N-BUTANE AT 100 PSIA
Bubblepoint T at fixed P                          Equation of state is : SRK

TEMPERATURE=  144.61 DEG F ,PRESSURE=  100.00 PSIA


FEED/PRODUCT RATES ARE LB-MOLS

COMPONENT        FEED            LIQUID           VAPOR        K
 NAME         MOLS MOL FR      MOLS MOL FR      MOLS MOL FR   VALUE

NC4H10       100.00 1.0000    100.00 1.0000       .00 1.0000   1.00000

TOTAL        100.00 1.0000    100.00 1.0000       .00 1.0000

H;KBTU       145.07  1.451    145.07  1.451       .00  9.518
S;KBTU/R       5.91   .059      5.91   .059       .00   .072
MOL WT       58.124           58.124           58.124
D;LB/FT3                      32.763            1.048
MASS;LB      5812.4           5812.4              .0
MOL % VAP=     .00;WT % VAP=     .00;VOL % LIQ=  100.00
LIQ COMPRESSIBILITY FACTOR = 0.03000  VAP COMPRESSIBILITY FACTOR = 0.856
```

Table A2

```
 This EZ*THERMO is licensed to:
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    CEC, Inc.
    June 23, 1997

BUBBLEPOINT OF N-BUTANE AT 100 PSIA
Bubblepoint T at fixed P                        Equation of state is : SRK

TEMPERATURE=  500.00 DEG F ,PRESSURE=  100.00 PSIA


FEED/PRODUCT RATES ARE LB-MOLS

COMPONENT         FEED            LIQUID            VAPOR        K
 NAME         MOLS MOL FR      MOLS MOL FR      MOLS MOL FR   VALUE

NC4H10       100.00 1.0000    100.00 1.0000       .00 1.0000   1.00000

TOTAL        100.00 1.0000    100.00 1.0000       .00 1.0000

H;KBTU      2099.26 20.993   2099.26 20.993       .00 20.993
S;KBTU/R      8.72   .087      8.72   .087       .00   .087
MOL WT       58.124           58.124           58.124
D;LB/FT3                      21.785             .581
MASS;LB      5812.4           5812.4              .0
MOL % VAP=      .00;WT % VAP=      .00;VOL % LIQ=  100.00
LIQ COMPRESSIBILITY FACTOR = 0.97190  VAP COMPRESSIBILITY FACTOR = 0.972
```

Table A3

```
 This EZ*THERMO is licensed to:
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    CEC, Inc.
    June 23, 1997

BUBBLEPOINT OF N-BUTANE AT 100 PSIA
Bubblepoint T at fixed P                          Equation of state is : SRK

TEMPERATURE=  144.61 DEG F ,PRESSURE=  100.00 PSIA


FEED/PRODUCT RATES ARE LB-MOLS

COMPONENT        FEED            LIQUID            VAPOR        K
 NAME         MOLS MOL FR      MOLS MOL FR      MOLS MOL FR   VALUE

NC4H10       100.00 1.0000    100.00 1.0000       .00 1.0000   1.00000
IC5H12         .00  .0000      .00  .0000       .00  .0000    .48921

TOTAL        100.00 1.0000    100.00 1.0000       .00 1.0000

H;KBTU       145.07  1.451    145.07  1.451       .00  9.518
S;KBTU/R       5.91   .059      5.91   .059       .00   .072
MOL WT       58.124           58.124           58.124
D;LB/FT3                      32.763            1.048
MASS;LB      5812.4           5812.4              .0
MOL % VAP=      .00;WT % VAP=      .00;VOL % LIQ=  100.00
LIQ COMPRESSIBILITY FACTOR = 0.03000  VAP COMPRESSIBILITY FACTOR = 0.856
```

Table A4

```
 This EZ*THERMO is licensed to:
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    CEC, Inc.
    June 23, 1997

BUBBLEPOINT OF N-BUTANE AT 100 PSIA
Bubblepoint T at fixed P                          Equation of state is : SRK

TEMPERATURE=  500.00 DEG F ,PRESSURE=  100.00 PSIA


FEED/PRODUCT RATES ARE LB-MOLS

COMPONENT          FEED              LIQUID             VAPOR        K
 NAME          MOLS MOL FR       MOLS MOL FR       MOLS MOL FR    VALUE

NC4H10       100.00 1.0000     100.00 1.0000        .00 1.0000    1.00000
IC5H12          .00  .0000        .00  .0000        .00  .0000    1.00000

TOTAL        100.00 1.0000     100.00 1.0000        .00 1.0000

H;KBTU      2099.26 20.993    2099.26 20.993        .00 20.993
S;KBTU/R       8.72   .087       8.72   .087        .00   .087
MOL WT       58.124             58.124            58.124
D;LB/FT3                        21.785              .581
MASS;LB      5812.4             5812.4               .0
MOL % VAP=      .00;WT % VAP=      .00;VOL % LIQ=  100.00
LIQ COMPRESSIBILITY FACTOR = 0.97190  VAP COMPRESSIBILITY FACTOR = 0.972
```

Table A5

```
 This EZ*THERMO is licensed to:
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    CEC, Inc.
    June 23, 1997

FLASH FOR 50% BUTANE - 50% PENTANE MIXTURE

Flash at fixed L/F and P                        Equation of state is : SRK

TEMPERATURE=  184.84 DEG F ,PRESSURE=  100.00 PSIA

FEED/PRODUCT RATES ARE LB-MOLS

COMPONENT        FEED           LIQUID          VAPOR        K
 NAME         MOLS MOL FR     MOLS MOL FR     MOLS MOL FR   VALUE

NC4H10        50.00  .5000     19.94  .3988     30.06  .6012   1.50782
NC5H12        50.00  .5000     30.06  .6012     19.94  .3988    .66321

TOTAL        100.00 1.0000     50.00 1.0000     50.00 1.0000

H;KBTU       731.77  7.318    156.60  3.132    575.17 11.503
S;KBTU/R       7.40   .074      3.42   .068      3.99   .080
MOL WT       65.137           66.558           63.717
D;LB/FT3                      33.259            1.075
MASS;LB      6513.7           3327.9           3185.8
MOL % VAP=   50.00;WT % VAP=   48.91;VOL % LIQ=    3.27
LIQ COMPRESSIBILITY FACTOR = 0.03211  VAP COMPRESSIBILITY FACTOR = 0.857
```

Table A6

This EZ*THERMO is licensed to:
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CEC, Inc.
June 23, 1997

FLASH FOR 50% BUTANE - 50% PENTANE MIXTURE

Flash at fixed L/F and P Equation of state is : SRK

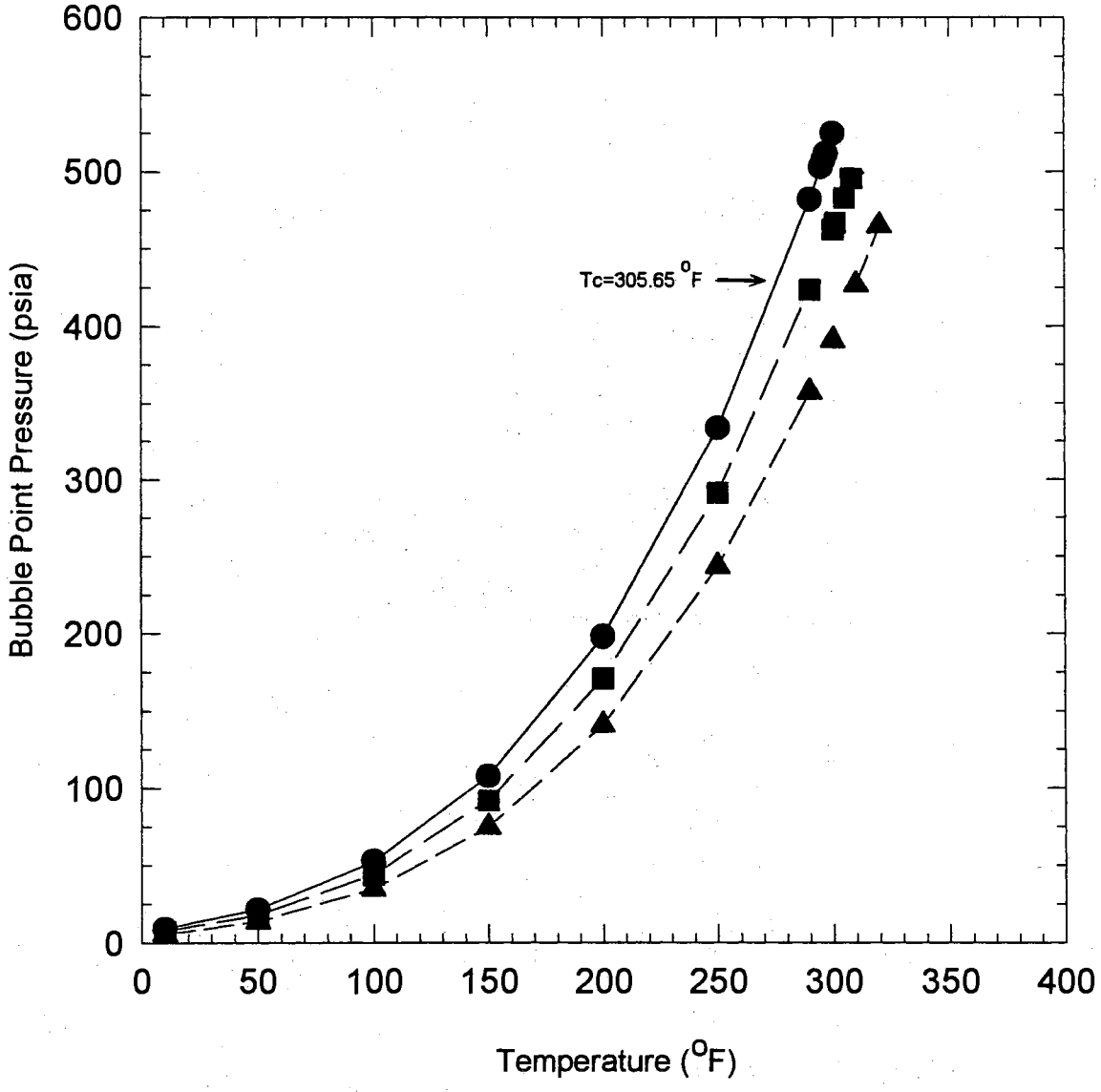
TEMPERATURE= 504.00 DEG F ,PRESSURE= 100.00 PSIA

FEED/PRODUCT RATES ARE LB-MOLS

COMPONENT NAME	FEED MOLS	FEED MOL FR	LIQUID MOLS	LIQUID MOL FR	VAPOR MOLS	VAPOR MOL FR	K VALUE
NC4H10	50.00	.5000	24.97	.4995	25.03	.5005	1.00218
NC5H12	50.00	.5000	25.03	.5005	24.97	.4995	.99786
TOTAL	100.00	1.0000	50.00	1.0000	50.00	1.0000	
H;KBTU	2332.59	23.326	1164.52	23.290	1168.07	23.361	
S;KBTU/R	9.53	.095	4.77	.095	4.77	.095	
MOL WT	65.138		65.145		65.130		
D;LB/FT3			22.090		.648		
MASS;LB	6513.8		3257.3		3256.5		

MOL % VAP= 50.00;WT % VAP= 49.99;VOL % LIQ= 2.85
LIQ COMPRESSIBILITY FACTOR = 0.95430 VAP COMPRESSIBILITY FACTOR = 0.972

Fiqure A1.


600
500
400
300
200
100
0
Bubble Point Pressure (psia)
Tc=305.65 °F
0
50
100
150
200
250
300
350
400
Temperature (°F)

VITA

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